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PTO/SB/21 (09-04)
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(to be used for all correspondence after initial filing)

Application Number	10/788,743
Filing Date	February 25, 2004
First Named Inventor	AKERS, Douglas W.
Art Unit	3663
Examiner Name	Palabrica, R.J.
Attorney Docket Number	B-200 (Ineel-112c)
Total Number of Pages in This Submission	181

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  - ☐ Fee Attached
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Signature	Bruce E Dahl		
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Date	July 21, 2006	Reg. No.	33,670

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Signature	Chasity Rossum		
Typed or printed name	Chasity C. Rossum	Date	July 21, 2006

IN THE UNITED STATES PATENT AND TRADEMARK OFFICE
BEFORE THE BOARD OF PATENT APPEALS AND INTERFERENCES

In Re Application of:	)	
	)	
AKERS, Douglas, W.	)	Examiner: Palabrica, R.J.
	)	
Serial No. 10/788,743	)	
	)	Group Art Unit: 3663
Filing Date: February 25, 2004	)	
	)	
For: METHOD FOR ON-LINE EVALUATION OF MATERIALS USING PROMPT GAMMA RAY ANALYSIS	)	Confirmation No.: 6111
	)	
Atty Dkt: B-200	)	

APPEAL BRIEF

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BEFORE THE BOARD OF PATENT APPEALS AND INTERFERENCES

In Re Application of:	)	
	)	
AKERS, Douglas, W.	)	Examiner: Palabrica, R.J.
	)	
Serial No. 09/932,531	)	
	)	Group Art Unit: 3641
Filing Date: August 17, 2001	)	
	)	
For: APPARATUS FOR PHOTON ACTIVATION POSITRON ANNIHILATION ANALYSIS	)	Confirmation No.: 4276
	)	
	)	
	)	
Atty Dkt: B-124	)	

APPEAL BRIEF

To: Commissioner of Patents
P.O. Box 1450
Alexandria, VA 22313-1450

Sir:

This Appeal Brief is submitted in response to the final rejections of the claims dated March 1, 2006. A Notice of Appeal was filed on May 24, 2006.

REAL PARTY-IN-INTEREST

The assignee of the entire right, title, and interest in the patent application is Bechtel BWXT Idaho, LLC.

RELATED APPEALS AND INTERFERENCES

There are three related appeals of other United States patent applications that may directly affect, or be directly affected by, or have a bearing on, the Board's decision. Divisional application, serial no. 10/269,807, filed October 10, 2003, came before the Board in Appeal No. 2005-0855. The Board mailed its decision to the appellant on May 31, 2005. United States Patent No. 7,058,153 subsequently issued on June 6, 2006. Divisional application, serial no. 10/383,096, filed March 5, 2003, is currently pending on appeal in the briefing stage. In parent application, serial no. 09/932,531, filed August 17, 2001, an appeal brief was filed on June 21, 2006. The current application is a continuation-in-part of parent application, serial no. 09/932,531, and a continuation-in-part of divisional application, serial no. 10/383,096.

There are currently no related interferences known to appellant, appellant's legal representative, or the assignee which will directly affect, or be directly affected by, or have a bearing on, the Board's decision.

STATUS OF THE CLAIMS

Claims 1-10, 12-19 and 21-23 are pending in the application. Claims 1-10, 12-19 and 21-23 currently stand rejected. The rejections of claims 1-10, 12-19 and 21-23 are appealed.

In the present application, the examiner provisionally rejected claim 2 under the judicially-created doctrine of double patenting over claim 3 of co-pending divisional application, serial no. 10/383,096. The appellant did not traverse this provisional rejection and has agreed to file the appropriate terminal disclaimer in the appropriate application at the appropriate time (i.e., upon the indication of allowance of either claim 2 in this application or claim 3 of the co-pending application).

STATUS OF AMENDMENTS

No amendments were filed or entered subsequent to the final office action mailed on March 1, 2006.

SUMMARY OF CLAIMED SUBJECT MATTER

The present invention is directed to a method for evaluating a material specimen by bombarding it with neutrons to create prompt gamma rays. The invention as claimed is summarized below with reference to the independent claims and claims separately argued. Claims 1 and 12 are independent claims. Claims 2, 13-19, 21 and 23 are dependent claims argued separately. The claims contain reference numerals and reference to the specification and drawings. All references are shown in the application at least where indicated herein.

1. A method (226; Fig. 9; ¶72) for evaluating a material specimen (12, 112, 212; Figs. 1, 7-9; ¶¶23-31, 33-34, 37-40, 43, 47, 50-53, 055-57, 59-63, 66, 68-69, 71-75, 77), comprising:

mounting (228, Fig. 9; ¶¶37, 59-61, 72-74, 77) a neutron source (14, 54, 114, 214, 254; Figs. 1, 7-9; ¶¶23-30, 32-34, 36-37, 50, 52, 56-63, 72-74, 77) adjacent the material specimen (12, 112, 212);

mounting (Fig. 9; ¶¶ 38, 40, 66-69) a detector (16, 30, 32, 116, 130, 216, 230; Figs. 1, 4, 6-9; ¶¶23-24, 36, 38-42, 44-46, 49, 52-54, 56, 60, 65-72, 74-77) adjacent the material specimen (12, 112, 212);

bombarding (232; Fig. 9; ¶¶23-24, 30-31, 34, 37, 50, 56, 59-61,73) the material specimen (12, 112, 212) with neutrons (Figs. 1, 7-9; ¶¶30-34, 37, 50, 52, 56-63, 73) from the neutron source (14, 114, 214) to create prompt gamma rays (Figs. 1, 7-9; ¶¶23-24, 27, 30, 34, 37-39, 41, 43-45, 49-53, 57, 60-61, 63, 66-67) within the material specimen (12, 112, 212), some of the prompt gamma rays being emitted from the material specimen (12, 112, 212), some of the prompt gamma rays resulting in the formation of positrons (Figs. 1, 7-9; ¶¶23-25, 27, 30-31, 34, 37, 43, 50-52, 56-57, 60-61, 63) within the material specimen

(12, 112, 212) by pair production (18, 218; Figs. 1, 7-9; ¶¶23, 28, 30-31, 37, 50, 52, 57, 60-61, 63);

collecting (70, 82, 234; Figs. 3, 6, 9; ¶75) positron annihilation data (22, 122, 222; Figs. 1, 3, 4, 6-9; ¶¶ 38, 42-45, 49, 53-54, 67, 70-71, 75-77) by detecting with the detector (16, 30, 32, 116, 130, 216, 230) a plurality of emitted annihilation gamma rays (Figs. 1, 7-9); ¶¶23-24, 30, 38-39, 41, 43, 45, 51-53, 57, 66-67) resulting from the annihilation (¶¶24, 30, 43-44, 57) of positrons, the detector (16, 30, 32, 116, 130, 216, 230) producing the positron annihilation data (22, 122, 222);

processing (84, 236; Figs. 6, 9; ¶¶26, 42, 47, 49, 53-54, 67, 70, 75, 77) collected positron annihilation data (22, 122, 222) in accordance with a Doppler-broadening algorithm (40; Figs. 2, 6; ¶¶26-27, 38, 42, 47-49, 51, 70, 75); and

continuing (238; Fig. 9; ¶75-76) to collect and process positron annihilation data (22, 122, 222) to measure an accumulation of lattice damage (¶¶24-26, 43, 47, 60-61, 67-69, 71, 74, 77) over time.

2. The method of claim 1, further comprising:

collecting (234; Fig. 9, ¶75-76) prompt gamma ray data (20, 120, 220; Figs. 1, 4, 7-9, ¶¶24-25, 38, 42-45, 49, 53-54, 67, 70-71, 75-77) by detecting with the detector (16, 30, 32, 116, 130, 216, 230) a plurality of emitted prompt gamma rays (Figs. 1, 7-9; ¶¶23-24, 27, 30, 34, 37-39, 41, 43-45, 49-53, 57, 60-61, 63, 66-67), the detector (16, 30, 32, 116, 130, 216, 230) producing the prompt gamma ray data (20, 120, 220);

calculating (72; Fig. 3; ¶¶25, 42-46, 51, 70) positron lifetime data (¶¶25, 27, 42-46, 51, 53, 70) from the positron annihilation data (22, 122, 222) and the prompt gamma ray data (20, 120, 220); and

continuing (238; Fig. 9; ¶¶75-76) to collect positron annihilation data (22, 122, 222) and prompt gamma ray data (20, 120, 220) and calculate (72) positron lifetime data to measure an accumulation of lattice damage over time.

12. A method for evaluating a material specimen (12, 112, 212; Figs. 1, 7-9; ¶¶23-31, 33-34, 37-40, 43, 47, 50-53, 055-57, 59-63, 66, 68-69, 71-75, 77), comprising:

mounting (228, Fig. 9; ¶¶37, 59-61, 72-74, 77) a neutron source (14, 54, 114, 214, 254; Figs. 1, 7-9; ¶¶23-30, 32-34, 36-37, 50, 52, 56-63, 72-74, 77) adjacent the material specimen (12, 112, 212);

mounting (Fig. 9; ¶¶ 38, 40, 66-69) a detector (16, 30, 32, 116, 130, 216, 230; Figs. 1, 4, 6-9; ¶¶23-24, 36, 38-42, 44-46, 49, 52-54, 56, 60, 65-72, 74-77) adjacent the material specimen (12, 112, 212);

bombarding (232; Fig. 9; ¶¶23-24, 30-31, 34, 37, 50, 56, 59-61,73) the material specimen (12, 112, 212) with neutrons (Figs. 1, 7-9; ¶¶30-34, 37, 50, 52, 56-63, 73) from the neutron source (14, 54, 114, 214, 254) to create prompt gamma rays (Figs. 1, 7-9; ¶¶23-24, 27, 30, 34, 37-39, 41, 43-45, 49-53, 57, 60-61, 63, 66-67) within the material specimen (12, 112, 212), some of the prompt gamma rays being emitted from the material specimen (12, 112, 212), some of the prompt gamma rays resulting in the formation of positrons (Figs. 1, 7-9; ¶¶23-25, 27, 30-31, 34, 37, 43, 50-52, 56-57, 60-61, 63) within the material specimen (12, 112, 212) by pair production (18, 218; Figs. 1, 7-9; ¶¶23, 28, 30-31, 37, 50, 52, 57, 60-61, 63);

collecting (70, 82, 234; Figs. 3, 6, 9; ¶75) positron annihilation data (22, 122, 222; Figs. 1, 3, 4, 6-9; ¶¶ 38, 42-45, 49, 53-54, 67, 70-71, 75-77) by detecting with the detector (16, 30, 32, 116, 130, 216, 230) a plurality of emitted annihilation gamma rays (Figs. 1, 7-9); ¶¶23-24, 30, 38-39, 41, 43, 45, 51-53, 57, 66-67) resulting from the annihilation (¶¶24,

30, 43-44, 57) of positrons, the detector (16, 30, 32, 116, 130, 216, 230) producing the positron annihilation data (22, 122, 222);

storing (¶¶ 71, 76) the positron annihilation data (22, 122, 222) on a data storage system (225; ¶¶ 71, 76) for later retrieval and processing; and

continuing to collect and store positron annihilation data (22, 122, 222), the continued collected and stored positron annihilation data (22, 122, 222) being indicative of an accumulation of lattice damage (¶¶24-26, 43, 47, 60-61, 67-69, 71, 74, 77) over time.

13. The method of claim 12, further comprising:

collecting prompt gamma ray data (20, 120, 220) by detecting with the detector (16, 30, 32, 116, 130, 216, 230) a plurality of emitted prompt gamma rays, the detector (16, 30, 32, 116, 130, 216, 230) producing the prompt gamma ray data (20, 120, 220) ;

storing prompt gamma ray data (20, 120, 220) on the data storage system (225) for later retrieval and processing; and

continuing to collect and store prompt gamma ray data (20, 120, 220) , the continued collected and stored prompt gamma ray (20, 120, 220) data being indicative of an accumulation of lattice damage over time.

14. The method of claim 12, wherein said mounting (228) a neutron source (14, 54, 114, 214, 254) adjacent the material specimen (12, 112, 212) comprises mounting (228) the neutron source (14, 54, 114, 214, 254) to the material specimen (12, 112, 212).

15. The method of claim 14, wherein said mounting a detector (16, 30, 32, 116, 130, 216, 230) adjacent the material specimen (12, 112, 212) comprises mounting the detector (16, 30, 32, 116, 130, 216, 230) to the material specimen (12, 112, 212).

16. The method of claim 15, further comprising positioning a shield (56, 256; Figs. 1, 8; ¶¶33, 62) adjacent the neutron source (14, 54, 114, 214, 254) to absorb stray neutrons.

17. The method of claim 16, further comprising positioning a moderator (60, 260; Figs. 1, 8; ¶¶34-36, 63-65) between the neutron source (14, 54, 114, 214, 254) and the material specimen (12, 112, 212).

18. The method of claim 12, wherein mounting (228) a neutron source (14, 54, 114, 214, 254) adjacent the material specimen (12, 112, 212) comprises mounting (228) an isotopic neutron source (54, 254) adjacent the material specimen (12, 112, 212).

19. The method of claim 12, wherein continuing to collect and store positron annihilation data (22, 122, 222) is performed while the material specimen (12, 112, 212) is in service.

21. The method of claim 12, further comprising:

retrieving stored positron annihilation data (22, 122, 222); and

processing (84, 236; Figs. 6, 9; ¶¶26, 42, 47, 49, 53-54, 67, 70, 75, 77) the positron annihilation data (22, 122, 222) in accordance with a Doppler-broadening algorithm (40; Figs. 2, 6; ¶¶26-27, 38, 42, 47-49, 51, 70, 75) to produce output data indicative of an accumulation of lattice damage over time.

23. The method of claim 12, further comprising removing the neutron source (14, 54, 114, 214, 254) before collecting positron annihilation data (22, 122, 222).

GROUNDS OF REJECTION TO BE REVIEWED ON APPEAL

1. Whether claims 1-10, 12-19 and 21-23 are patentable under 35 U.S.C. §112, first paragraph, as complying with the enablement requirement.

2. Whether claims 1-10, 12-19 and 21-23 are patentable under 35 U.S.C. §112, second paragraph, as distinctly claiming the subject matter of the invention.

ARGUMENT

Opening Statement

By virtue of the examiner's rejections, this appeal once again raises virtually the same issues that the Board has already decided, yet must decide again here (as well as, in the appeal of application serial nos. 09/932,531 and 10/383,096). Once again, the examiner has rejected all the claims in this application for indefiniteness and lack of enablement. Yet, in his quest to brand all the claims indefinite and not enabled, he has based his rejections primarily on limitations that are not part of the claims at issue in *this* application. However, even where the examiner's rejections were actually tied to claim limitations requiring use of a Doppler-broadening algorithm, for example, those claims are enabled and sufficiently definite. The Board reached the same conclusion in a related case, reversing this examiner's rejections of lack of enablement and indefiniteness. The Board's words apply equally well here:

> [W]hile the appellant's disclosure does not convey much detail as to the various algorithms described therein, these algorithms admittedly are generally known in the art. The examiner has failed to advance any cogent reasoning as to why the disclosure would not have enabled a person of ordinary skill in the art to employ these algorithms without undue experimentation.

Ex parte Akers, Appeal No. 2005-0855, at 8 (Bd. Pat. App. & Interf. 2005) (slip op.). The Board also reversed the examiner's rejections based on indefiniteness of the claims as follows:

> The examiner views the appealed claims to be indefinite for reasons essentially similar to those listed above in connection with the enablement rejection. In this regard, the examiner points to the claim limitations relation to . . . the positron lifetime, Doppler-broadening, three-dimensional imaging and activation/analysis process algorithms. . . . . [T]he examiner's criticism of the claim limitations pertaining to the algorithms . . . focus[es]on the breadth of these limitations. It is well settled, however, that mere breadth does not equate to indefiniteness. In re Miller, 441 F.2d 689, 169 USPQ 597, 600 (CCPA 1971).

Id. at 9. Thus, the examiner's rejections should be reversed.

I. Whether claims 1-10, 12-19 and 21-23 are patentable under 35 U.S.C. §112, first paragraph, as complying with the enablement requirement.

A. Legal Standard For Rejecting Claims Under 35 U.S.C. §112, First Paragraph

The legal standard for determining whether the disclosure provides a sufficient description of the invention is whether a person reasonably skilled in the art could make or use the invention without undue experimentation based on the disclosure and on information known in the art. *United States v. Telectronics, Inc.*, 857 F.2d 778, 8 USPQ2d 1217 (Fed. Cir. 1988). The fact that experimentation may be complex does not necessarily make it undue if the art typically engages in such experimentation. *In re Wands*, 858 F.2d 731, 8 USPQ2d 1400 (Fed. Cir. 1988). *See Ex parte Lemelson,* 2002 WL 32334419, *3 (Bd. Pat. App. & Interf. 2002) ("The fact that an invention is sophisticated and complex does not, by itself, lead to the conclusion that undue experimentation would be required to make and use the invention.") That is, the test of enablement is not whether any experimentation is required, but whether, if experimentation is necessary, it is undue. *In re Angstadt*, 537 F.2d 498, 190 USPQ 214 (CCPA 1976).

The factors to be considered when determining whether a claim limitation is enabled and whether any necessary experimentation is "undue" include, but are not limited to: (1) the breadth of the claims; (2) the nature of the invention; (3) the state of the prior art; (4) the level of one of ordinary skill; (5) the level of predictability in the art; (6) the amount of direction provided by the inventor; (7) the existence of working examples; and (8) the quantity of experimentation needed to make or use the invention based on the content of the disclosure. *In re Wands*, 858 F.2d at 737; MPEP 2164.01(a). It is improper to conclude that a disclosure is not enabling based on an analysis of only one of the above factors while ignoring one or more of the others. *See, e.g., Ex parte Noguchi,* 2002 WL

1801470 (Bd. Pat. App. & Interf. 2002) (supplying information directed to one factor is insufficient); *Ex parte Kopetzki*, 2001 WL 11197754 (Bd. Pat. App. & Interf. 2001) (merely reciting facts without reference to the factors is insufficient); MPEP 2164.01(a). Moreover, whether the specification is enabling must be determined with reference only to the limitations claimed. *CFMT, Inc. v. Yieldup Int'l Corp.*, 349 F.3d 1333, 1338 (Fed. Cir. 2003).

With regard to the burden of proof required to support a rejection under §112, the Patent Office is required to assume that the specification complies with the enablement provision of §112 unless it has acceptable evidence or reasoning to suggest otherwise. *See, e.g., In re Marzocchi*, 439 F.2d 220, 169 USPQ 367 (CCPA 1979). The Patent Office thus must provide reasons, supported by the record as a whole, why the specification is not enabling. Then and only then does the burden shift to the applicant to show that one of ordinary skill in the art could have practiced the claimed invention without undue experimentation. *Gould v. Missinghoff*, 229 USPQ 1 (D.D.C. 1985), *aff'd in part, vacated in part, and remanded sub. nom., Gould v. Quigg*, 822 F.2d 1074, 3 USPQ2d 1302 (Fed. Cir. 1987). Mere conclusionary statements as to the level of ordinary skill in the art are not a sufficient basis for a rejection under 35 U.S.C. §112. *In re Brebner*, 455 F.2d 1402, 173 USPQ 169 (CCPA 1972). In addition, the law does not require, and indeed prefers, that a patent specification omit that which is well-known. *In re Buchner*, 929 F.2d 660, 18 USPQ2d 1331 (Fed. Cir. 1991).

B. Response to Examiner's Rejections

The examiner failed to carry his prima facie burden of demonstrating that claims 1-10, 12-19 and 21-23 are not enabled as required by §112, first paragraph. First, the examiner's rejections are based on limitations that are not part of the claims. Second, where the examiner did base his rejections on at least one limitation actually contained in

the claims, the examiner failed to analyze the enablement issue with reference to the eight required factors. Finally, given that Doppler-broadening (and other) algorithms are well-known in the art, the level of detail contained in the specification sufficiently enables the claims.

1. Rejections are improperly based on limitations not in the claims.

As an initial matter, the examiner argues that "the claims require the use of algorithms (i.e., Doppler-broadening and positron lifetime), detector(s), a neutron source and a data processor. Thus to enable an artisan to make and use an operative embodiment, one must first know which particular algorithm(s) to use, and how and in what manner the data from the detectors are to be analyzed in the data processor." Final Office Action at 2. A fundamental deficiency in the examiner's argument is that none of the claims requires use of a data processor. And, none of the claims requires use of a positron lifetime algorithm. Since the examiner's rejections are based on limitations not found in the claims, they should be revised.

a. Independent claim 12 and dependent claims 13-19 and 23

Independent claim 12 and dependent claims 13-19 and 23 require neither processing in accordance with an algorithm nor use of a data processor. Therefore, the examiner's §112 rejections of these claims for lack of enablement of those limitations are improper on their face and should be reversed on that ground alone.

b. Independent claim 1 and dependent claims 2 and 21

Now the appellant turns to independent claim 1 and dependent claim 21, both of which contain the limitation, "processing . . . in accordance with a Doppler-broadening algorithm." Claim 2 claims the method of claim 1 further comprising "calculating positron lifetime data;" however, claim 2 does not require use of a positron lifetime algorithm. The examiner argues that the claims are not enabled because undue

experimentation is necessary to select algorithms (including Doppler-broadening, positron lifetime, 3D imaging and selective activation algorithms) that will (1) obtain accurate detection of lattice defects (i.e., not too few and not too many); (2) obtain reasonable statistical analyses; (3) determine which algorithm (in conjunction with selection of "a suitable data processor") "actually provides a reasonable determination of the presence of enough lattice defects to be of concern;" and (4) determine "whether there are present enough lattice defects to cause metal fatigue, etc. . . . ." Final Office Action, p. 6. The examiner further argues that the appellant has failed to explain "how these algorithms have to be combined," referring to Doppler-broadening and positron lifetime algorithms. However, these limitations are not in the claims and, therefore cannot be considered when determining whether the specification enables the claims.

None of these claims requires a data processor; positron lifetime, 3-D imaging or selective activation algorithms; accuracy; reasonable statistical analysis; "provid[ing] a reasonable determination of the presence of enough lattice defects to be of concern;" or determining "whether there are present enough lattice defects to cause metal fatigue." Similarly, none of the claims requires combining Doppler-broadening and positron lifetime algorithms. As the Federal Circuit has held, "Title 35 does not require that a patent disclosure enable . . . a perfected, commercially viable embodiment absent a claim limitation to that effect." *CFMT, Inc. v. Yieldup Int'l Corp.*, 349 F.3d 1333, 1338 (Fed. Cir. 2003). Therefore, the examiner cannot evaluate enablement based on limitations not contained in the claims. *Id.*, 349 F.3d at 1338 (since claims contained no standard for cleanliness, claims for cleaning methods were enabled for any level of contaminant removal); *Ex parte Lemelson,* 2002 WL 32334419, *4.

c. Figure 2

Similarly, but without reference to any claims, the examiner objects to the

sufficiency of the disclosure in Figure 2, regarding a feedback arrangement between the data processing system 24 and the algorithms 38, 40. Final Office Action, p. 8. However, the examiner has not tied these arguments to the elements of any claim to show how such elements are not enabled. *CFMT, Inc.*, 349 F.3d at 1338 (level of disclosure necessary for enablement varies with the scope of the claims). Therefore, the examiner's arguments in this regard cannot be used to demonstrate a prima facie case of non-enablement.

d. *Ex parte Lemelson*

The case of *Ex parte Lemelson,* 2002 WL 32334419, presents similar facts to the ones here and is persuasive in its analysis of enablement. In that case, the invention was directed to a method and apparatus for controlling the travel of a powered vehicle, comprising calculating whether the vehicle and an object are on a collision course by measuring the distance to and relative velocity between the two, and using fuzzy logic interference rules to determine a combination of steering and acceleration to avoid a collision. The examiner rejected the claims for lack of enablement on grounds almost identical to the ones here:

> The rejection also states that the disclosure is insufficient for teaching how to distinguish one object from another object or how to determine distance and relative velocity of each object. . . . The examiner observes that the object detection and recognition and the fuzzy logic rules require complex algorithms and extensive processing that are not sufficiently described in the disclosure [citation omitted]. In the final rejection the examiner added that the complexity of putting all the features into one real-time system required undue experimentation.

Id., at *2. The appellants argued that fuzzy logic and image analysis were techniques well-known in the art. The Board reversed the examiner's rejections. First, the Board held that the examiner improperly based his rejections on a real-time operation requirement not included in the claims. It also held, "Second, the examiner's findings of undue experimentation are mere conclusions based on the examiner's own speculations.

The examiner essentially finds that there would be undue experimentation because the claimed invention requires sophisticated and complex operations. The fact that an invention is sophisticated and complex does not, by itself, lead to the conclusion that undue experimentation would be required to make and use the invention." *Id.* at *3. The Board's analysis applies equally well here, demonstrating that the examiner failed to carry his burden.

e. Dependent claims 2-10 and 22

In addition, claims 2-10 and 22 depend from claim 1 and are also allowable at least for the reasons that claim 1 is allowable.

2. <u>The eight required factors were not addressed</u>.

While the examiner sets forth a laundry list of variables that he argues one of ordinary skill in the art must consider when choosing an appropriate Doppler-broadening algorithm, positron lifetime algorithm, or other algorithm, the examiner has nonetheless failed to meet his prima facie burden. As an initial matter, again, (with the exception of Doppler-broadening) none of the claims at issue here requires processing in accordance with positron lifetime or other algorithms, so those "limitations" may not be considered in determining whether the claims are enabled. In addition, the examiner failed to undertake the required analyses to demonstrate lack of enablement.

Only claims 1 and 21 contain a limitation that the examiner argues was not enabled. That limitation is "processing . . . in accordance with a Doppler-broadening algorithm. As stated above, while claim 2 claims "calculating positron lifetime data," it does not require use of a positron lifetime algorithm. However, in rejecting claims 1, 2 and 21 (as well as all the other claims) for non-enablement, the examiner was required to analyze each of the eight required factors set forth in *In re Wands*, 858 F.2d 731, 737 (Fed. Cir. 1988), with reference to the claims, which he did not. Nor did the examiner supply

facts to support each and every factor required by *In re Wands*. The Board has repeatedly reversed similar rejections, holding that the examiner failed to meet his prima facie burden. *See, e.g., Ex parte Noguchi*, 2002 WL 1801470 (Bd. Pat. App. & Interf. 2002) (supplying information directed to one factor is insufficient); *Ex parte Kopetzki*, 2001 WL 11197754 (Bd. Pat. App. & Interf. 2001) (merely reciting facts without reference to the factors is insufficient). Even assuming that the examiner put forth any "facts" (which is denied), the "mere citing of a series of facts, without relating them to the criteria for determining undue experimentation set forth in *In re Wands*, is not sufficient to establish a prima facie case of nonenablement." *Ex parte Kopetzki*, 2001 WL 11197754, at *3. In addition, by reviewing the variables that one of ordinary skill in the art would know to consider, the examiner makes appellant's point that one of ordinary skill in the art would well know how to pick a suitable Doppler-broadening algorithm (or positron lifetime algorithm, assuming one were even required) and select appropriate constants, making any experimentation routine and not undue.

3. <u>The specification is enabling</u>.

Finally, given that Doppler-broadening algorithms are well-known, the level of detail provided in the present specification is sufficiently enabling, as the Board determined with reference to the appeal in the divisional case issued as U.S. Patent No. 7,058,153. *See supra* at p. 12. Moreover, even if a positron lifetime algorithm were required by claim 2 (which is denied), positron lifetime algorithms are also well-known, rendering the level of detail provided in the specification enabling as to that limitation, too.

The appellant specifically states in the specification that the Doppler-broadening algorithms and positron lifetime algorithms are well-known in the art and could be readily implemented by persons having ordinary skill in the art after having become familiar with

the teachings of the present invention. Specification, ¶¶ [0043]-[0049]. Because these algorithms are well-known to those of ordinary skill in the art who are familiar with their applications, the specification need not and does not describe them further. At no time has the examiner ever disputed the fact that these algorithms are well-known. Since that fact is undisputed, the examiner was bound to establish that the amount of experimentation in using these algorithms familiar to those of ordinary skill in the art would be undue. As explained above, he failed to make such a showing because he did not analyze the undue experimentation factors from *In re Wands*.

During prosecution, the appellant provided examples of issued patents to show the general level of detail required to enable similar inventions for those of ordinary skill in the art. *See* Amendment (1/13/06), p. 12. In his Summary of Argument presented in the appellant's Amendment dated January 13, 2006, the appellant stated that "the best measure of level of disclosure required in this particular field of endeavor can be obtained by reviewing issued U.S. patents in the same field." Amendment (1/13/06), p. 7. The examiner argued that U.S. Patent No. 6,178,218 to Akers ("Akers") and U.S. Patent No. 4,064,438 to Alex, et al. ("Alex") cannot be used by analogy to show the appropriate level of detail required for enablement. Final Office Action, p. 9. However, the examiner's arguments are not well-founded.

Specifically, the examiner argued that Akers cannot be used because his Doppler-broadening algorithm "is not modified by feed back from the data processing system. . . ." Final Office Action, p. 9. However, the claims at issue in this appeal do not contain as limitations either use of a data processing system or modification of the Doppler-broadening algorithm through feedback. Basing non-enablement rejections on limitations not found in the claims is improper.

Further, the examiner argues that Alex cannot be used to demonstrate enablement

by analogy because Alex uses a positron lifetime algorithm for a different purpose than do the claims of the present invention. As an initial matter, none of the claims at issue here requires use of a positron lifetime algorithm. While claim 2 claims "calculating positron lifetime data," it does not require use of a positron lifetime algorithm. In any event, the examiner misses the point. The point is that the description in Alex enables his claim limitation of a method "wherein the variations in annihilation characteristics within the tested material are detected by positron lifetime measurements." The description of positron lifetime measurements in Alex contains even less detail than the present specification, merely referring to one page of a previously published book and one issued patent. *Compare* Alex, Col. 6, lns. 60-66 *with* Specification ¶¶ [0043]-[0046]. If such a brief description in Alex were considered enabling, then the more detailed description of the present specification must also be considered enabling to one of ordinary skill in the art. Finally, the other references previously cited by the examiner (i.e., Derlet, Bandžuch, Zhu, and Shaffer) illustrate that persons having ordinary skill in the art are well-aware of the appropriate use and description of Doppler-broadening and positron lifetime algorithms, as well as the various issues and complexities involved in selecting, modifying and combining any of these algorithms, rendering any experimentation required routine and not undue.

The examiner argues that "the specification indicates that there are different known Doppler-broadening algorithms <u>but</u>, fails to disclose <u>which</u> of these known algorithms would be suitable for use in the present invention." Final Office Action, p. 3. That is not the case. The specification specifically discloses a suitable algorithm when it states that "in one preferred embodiment of the invention, the Doppler-broadening algorithm 40 may comprise the Doppler-broadening algorithm described in U.S. Patent No. 6,178,218 B1 . . . ." Specification ¶[0048]. Contrary to the examiner's suggestion, there is no

experimentation involved at all in selecting the precise algorithm the appellant identified in the specification.

The examiner reads the specification as requiring that "both the positron lifetime algorithm and Doppler-broadening algorithm, each requires two detectors." Final Office Action, p. 8. He then states the specification also discloses that one detector may be used. Without reference to any limitations in the claims, the examiner argues that appellant's "disclosure is thus clearly insufficient and non-enabling as to which specific known positron lifetime algorithm can be used with only a single detector and, which specific Doppler-broadening algorithm can be used with only a single detector." *Id.* at p. 8. The appellant understands the examiner to be arguing that the embodiment using a single detector is not enabled. However, the examiner's argument is incorrect because the claims are not limited to the use of one detector.

Independent claims 1 and 12 claim a "method for evaluating a material specimen, comprising . . . *a* detector . . . ." (Emphasis added.) The Federal Circuit could not have been more clear when it cautioned, "This court has repeatedly emphasized that an indefinite article 'a' or 'an' in patent parlance carries the meaning of 'one or more" in open-ended claims containing the transitional phrase, 'comprising.'" *KCJ Corp. v. Kinetic Concepts, Inc.*, 223 F.3d 1351, 1356 (Fed. Cir. 2000). The Federal Circuit then stated, "Moreover, standing alone, a disclosure of a preferred or exemplary embodiment encompassing a singular element does not disclaim a plural embodiment." *Id.* at 1356. Thus, in accordance with the holding of the Federal Circuit, use of the article "a" in conjunction with the word "detector" and the transitional phrase "comprising" means that the claims set forth above comprise "one or more" detectors. The specification enables the use of "one or more" detectors. While the specification notes that two detectors may be preferred, this does not operate to exclude one detector either. Moreover, even if the

examiner were correct that the specification enabled only the use of two detectors (which is denied), the scope of all the claims covers two (i.e., one or more) detectors. Since one embodiment covered by the claim is enabled, then the enablement requirement is satisfied. The words of the Board in another case cannot be improved upon: "The examiner's reasoning is logical but not entirely consistent with the law: enabling the 'full scope' of a claim does not necessarily require enabling every embodiment within the claim." *Ex parte Saito*, 2005 WL 3524580, *3 (Bd. Pat. App. & Interf. 2005).

Thus, the level of detail set forth in the specification is sufficiently enabling for one of ordinary skill in the art. Claims 2-10 and 22 ultimately depend from claim 1 and are also allowable at least for the reasons that claim 1 is allowable. Claims 13-19, 21 and 23 ultimately depend from claim 12 and are also allowable at least for the reasons that claim 12 is allowable.

Having failed (1) to base his rejections on limitations in the claims and (2) to analyze the *In re Wands* factors, the examiner failed to meet his prima facie burden to demonstrate that the claims are not enabled. In any event, as the Board previously determined with reference to a related case, descriptions of the various algorithms used in detecting positron annihilation events are sufficiently enabling.

II. Whether claims 1-10, 12-19 and 21-23 are patentable under 35 U.S.C. §112, second paragraph, as distinctly claiming the subject matter of the invention.

A. Legal Standard For Rejecting Claims Under 35 U.S.C. §112, Second Paragraph

Section 112, second paragraph, requires that the claims particularly point out and distinctly claim what the applicant regards as his invention. 35 U.S.C. § 112. The standard is one of reasonably particularity and completeness. MPEP 2173.02. "The indefiniteness inquiry focuses on whether those skilled in the art would understand the scope of the claim when the claim is read in light of the rest of the specification." *Union*

Pacific Res. Co. v. Chesapeake Energy Corp., 236 F.3d 684, 691 (Fed. Cir. 2001); *Credle v. Bond*, 25 F.3d 1566, 1576 (Fed. Cir. 1994) (all that is required under § 112, ¶2 is that one of ordinary skill in the art would understand the claim language based on the specification and the drawings). The degree of precision necessary for adequate claims depends on the nature of the subject matter. *Miles Laboratories, Inc., v. Shandon, Inc.*, 27 USPQ2d 1123 (Fed. Cir. 1993). As such, the Patent Office does not permit *per se* rejections of certain language as being indefinite under § 112, ¶ 2. MPEP 2173.02 ("Office policy is not to employ *per se* rules to make technical rejections.")

The examiner bears the initial burden of presenting evidence or reasoning to explain why persons skilled in the art would not understand the claim language based on the specification. *See In re Oetiker*, 977 F.2d 1443, 1445 (Fed. Cir. 1992). To meet that burden of proof, the MPEP requires that "[d]efiniteness of claim language *must* be analyzed, not in a vacuum, but in light of:

(A) The content of the particular application disclosure;

(B) The teachings of the prior art; and

(C) The claim interpretation that would be given by one possessing the ordinary level of skill in the pertinent art at the time the invention was made." MPEP 2173.02 (emphasis added). *See In re Johnson*, 558 F.2d 1008, 1015, 194 USPQ 187 (CCPA 1977). In addition, the Federal Circuit has repeatedly held that the enablement requirement and the written description requirement of 112 are not to be conflated. "We interpret 35 U.S.C. §112, ¶1 to require a written description requirement separate and apart from the enablement requirement." *In re Curtis*, 354 F.3d 1347, 1357 (Fed. Cir. 2004). *See In re Hyatt*, 708 F.2d 712, 715 (Fed. Cir. 1983) (the fact that a claim is not enabled does not render it indefinite). "After evidence or argument is submitted by the applicant in

response, patentability is determined on the totality of the record with due consideration to persuasiveness of argument." *In re Oetiker*, 977 F.2d at 1445.

B. Response to Examiner's Rejections

The examiner never established a prima facie case of indefiniteness. Indeed, the examiner's rejections here are indefinite, not the appellant's claim language. In short, by confusing breadth with indefiniteness, the examiner has issued improper rejections under §112, second paragraph. Moreover, even assuming that the examiner did carry his initial burden (which is denied), the appellant demonstrated that the claim language is definite, which evidence the examiner ignored. The indefiniteness rejections should be reversed.

1. The only specific rejection was traversed.

The only specific claim language that the examiner rejected during prosecution was "at least one" emitted gamma ray, which he rejected as indefinite in his office action of May 10, 2005. Claims previously containing that limitation have all been amended to "a plurality of" emitted gamma rays, thereby traversing the examiner's indefiniteness rejection. The examiner acknowledged that this rejection had been traversed in his October 17, 2005 office action. Despite this acknowledgement, in the same October 17, 2005 office action, the examiner newly rejected all of the claims as "vague and indefinite" without even specifying which claim language would not be understood by one of ordinary skill in the art. In the final office action, the examiner summarily dismissed the appellant's argument and evidence regarding definiteness as "not convincing" and merely incorporated by reference his previous action of October 17, 2005 which incorporated his previous action of May 10, 2005 which incorporated his arguments directed to the enablement issue.

The only specific rejection having been traversed, the examiner's rejection for indefiniteness should be reversed on those grounds alone.

2. <u>The examiner failed to meet his prima facie burden</u>.

Once his initial indefiniteness rejection was traversed, the examiner never specifically and directly identified the claim language that he considered "vague and indefinite." Rather, as stated above, he just bootstrapped his indefiniteness rejections onto his lack of enablement rejections. The examiner's indefinite rejections are therefore improper.

Not only did he fail to identify any deficient claim language, but also the examiner failed to perform the indefiniteness analyses required by MPEP 2173.02. For example, since the examiner never identified the claim language at issue, he certainly did not interpret the claim language, as required by the MPEP. Further the examiner has not provided any persuasive reasoning why any specific claim language is vague and indefinite.

Even assuming that such language were specified, by relying only on arguments he made to support his non-enablement rejections to support his indefiniteness rejections, the examiner failed to carry his burden. Indeed, the Federal Circuit has specifically stated, "[I]f the 'enabling' disclosure of a specification is not commensurate in scope with the subject matter encompassed by a claim, that fact does not render the claim imprecise or indefinite or otherwise not in compliance with the *second* paragraph of §112; rather the claim based on an *insufficient disclosure* (§112, first paragraph) and should be rejected on that ground." *In re Hyatt*, 708 F.2d at 715.

Having been based entirely on his non-enablement rejections, appellant therefore believes that the examiner's indefiniteness rejections extend to the scope of the Doppler-broadening algorithm claim limitation of claims 1 and 21, as well as claims 2-10 and 22 which depend from claim 1. (The appellant has already explained the error in the examiner's non-enablement rejections, having been based on limitations not found in the

claims. *See supra* at pp. 15-17). However, the examiner's rejections of all the claims as indefinite cannot be affirmed on that basis.

a. Independent claim 12 and dependent claims 13-19 and 23

First, claims 12-19 and 23 do not require the use of any algorithm and the examiner has put forth no evidence or reasoning as to why any specific claim limitation of those claims is imprecise. Having made out no case whatsoever that any language in claims 12-19 and 23 is indefinite, the examiner's rejections in that regard must be reversed.

b. Independent claim 1 and dependent claim 21

Second, with respect to the indefiniteness rejections of claim 1 (and its dependent claims 2-10 and 22) and claim 21 presumably based on the use of a Doppler-broadening algorithm, the words of the Board in the related appeal apply just as well here: "[T]he examiner's criticisms of the claim limitations pertaining to the algorithms . . . focus on the breadth of those limitations. It is well settled, however, that mere breadth does not equate to indefiniteness. In re Miller, 441 F.2d 689, 169 USPQ 597, 600 (CCPA 1971). Accordingly, the examiner's contention that the appealed claims are indefinite is unpersuasive." *Ex parte Akers, supra*, at 9-10.

3. The examiner failed to consider evidence of definiteness.

a. Independent claim 1 and dependent claims 2 and 21

Although the examiner never identified the specific claim language he considered to be indefinite, the applicant surmised that his rejections must have related to the claims language "processing . . . in accordance with a Doppler-broadening algorithm" (claims 1 and 21) and "calculating positron lifetime data" (claim 2). (Neither of these terms is present in independent claim 12 or claims 13-19 and 23). Based on that understanding, the appellant responded with evidence and argument, explaining why the "various algorithms

are not vague [or] indefinite . . . i.e., a the person having ordinary skill in the art would understand the algorithms and possess the knowledge required to evaluate the many algorithms available and select those that would be appropriate for the desired application." Amendment (1/13/06), p. 13. Such evidence and argument demonstrated that the examiner's rejections did not meet his prima facie burden.

Specifically, the appellant argued in his Amendment (1/13/06), pp. 12-13 that the claim language was not indefinite because:

(i) Persons having ordinary skill in the art would understand the algorithms and possess the knowledge required to evaluate the many algorithms available and select those that would be appropriate for the desired application.

(ii) With regard to the Doppler-broadening algorithm, the written description clearly states that several different types of Doppler-broadening techniques have been developed and could be used. The written description also states that the Doppler-broadening algorithm may comprise the algorithm disclosed in U.S. Patent No. 6,178,218.

(iii) The written description specifically states that systems for detecting positron lifetimes, as well as the algorithms utilized thereby, are well-known in the art and could be easily provided by persons having ordinary skill in the art after having become familiar with the teachings of the present invention.

Instead of addressing these arguments and presenting evidence why persons of ordinary skill in the art would not understand the meaning the claim terms set forth above, the examiner pronounced the arguments "not convincing." Final Office Action at p. 2. Without any further explanation, he merely incorporated his previous rejections by reference into his final office action. Final Office Action (3/1/06) at p. 12. In a similar situation where, in the examiner's answer, the examiner responded that the appellants'

arguments were "not persuasive," the Board held that the examiner failed to satisfy his burden. *See Ex parte Voordum*, 2002 WL 1801166, *4 (Bd. Pat. App. & Interf. 2002).

Even assuming that the examiner had specified the claim language set forth above as indefinite (which is denied), one of ordinary skill in the art would well understand the "processing . . . in accordance with a Doppler-broadening algorithm" (claims 1 and 21) and "calculating positron lifetime data" (claim 2). The examiner has failed to carry his burden to demonstrate otherwise.

Claims 3-10 and 22 depend from claim 1 and are allowable at least for the reasons that claim 1 is allowable.

b. Independent claim 12 and dependent claims 13-19 and 23

As mentioned above, claims 12-19 and 23 contain no limitations directed to any algorithmic claim limitation that the examiner evidently considers indefinite. Therefore, having failed to raise any specter that these claims are indefinite, the examiner's rejections as to these claims should be summarily reversed.

CONCLUSION

The principal deficiency in the examiner's rejections comes in his own lack of precision. He adhered neither to the specific language of the claims nor to the specific requirements of the MPEP in making his § 112 rejections. With respect to non-enablement, the examiner's rejections were largely based on limitations not found in the claims. Moreover, with respect to any limitations actually found in the claims, the examiner failed to perform the enablement analyses required by *In re Wands*, *supra*. With respect to indefiniteness, the examiner failed to identify any specific claim language that he considered to be indefinite. Moreover, merely piggybacking indefiniteness rejections on non-enablement rejections is improper, as the Federal Circuit has held. Thus, the

examiner's inability to (1) issue rejections based on language actually in the claims and (2) issue those rejections only after performing the analyses required by the MPEP is fatal to his rejections. The rejections for non-enablement and indefiniteness should be reversed.

Respectfully submitted,
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Date: July 21, 2006

CLAIMS APPENDIX

1. A method for evaluating a material specimen, comprising:

mounting a neutron source adjacent the material specimen;

mounting a detector adjacent the material specimen;

bombarding the material specimen with neutrons from the neutron source to create prompt gamma rays within the material specimen, some of the prompt gamma rays being emitted from the material specimen, some of the prompt gamma rays resulting in the formation of positrons within the material specimen by pair production;

collecting positron annihilation data by detecting with the detector a plurality of emitted annihilation gamma rays resulting from the annihilation of positrons, the detector producing the positron annihilation data;

processing collected positron annihilation data in accordance with a Doppler-broadening algorithm; and

continuing to collect and process positron annihilation data to measure an accumulation of lattice damage over time.

2. The method of claim 1, further comprising:

collecting prompt gamma ray data by detecting with the detector a plurality of emitted prompt gamma rays, the detector producing the prompt gamma ray data;

calculating positron lifetime data from the positron annihilation data and the prompt gamma ray data; and

continuing to collect positron annihilation data and prompt gamma ray data and calculate positron lifetime data to measure an accumulation of lattice damage over time.

3. The method of claim 1, wherein said mounting a neutron source adjacent the material specimen comprises mounting the neutron source to the material specimen.

4. The method of claim 3, wherein said mounting a detector adjacent the material specimen comprises mounting the detector to the material specimen.

5. The method of claim 4, further comprising positioning a shield adjacent the neutron source to absorb stray neutrons.

6. The method of claim 5, further comprising positioning a moderator between the neutron source and the material specimen.

7. The method of claim 6, further comprising positioning a reflector adjacent the neutron source to reflect neutrons toward the material specimen.

8. The method of claim 1, wherein mounting a neutron source adjacent the material specimen comprises mounting an isotopic neutron source adjacent the material specimen.

9. The method of claim 8, wherein mounting an isotopic neutron source adjacent the material specimen comprises mounting a neutron source of ^{252}Cf.

10. The method of claim 1, wherein continuing to collect and process positron annihilation data to measure an accumulation of lattice damage over time is performed while the material specimen is in service.

11. (Canceled).

12. A method for evaluating a material specimen, comprising:

mounting a neutron source adjacent the material specimen;

mounting a detector adjacent the material specimen;

bombarding the material specimen with neutrons from the neutron source to create prompt gamma rays within the material specimen, some of the prompt gamma rays being emitted from the material specimen, some of the prompt gamma rays resulting in the formation of positrons within the material specimen by pair production;

collecting positron annihilation data by detecting with the detector a plurality of emitted annihilation gamma rays resulting from the annihilation of positrons, the detector producing the positron annihilation data;

storing the positron annihilation data on a data storage system for later retrieval and processing; and

continuing to collect and store positron annihilation data, the continued collected and stored positron annihilation data being indicative of an accumulation of lattice damage over time.

13. The method of claim 12, further comprising:

collecting prompt gamma ray data by detecting with the detector a plurality of emitted prompt gamma rays, the detector producing the prompt gamma ray data;

storing prompt gamma ray data on the data storage system for later retrieval and processing; and

continuing to collect and store prompt gamma ray data, the continued collected and stored prompt gamma ray data being indicative of an accumulation of lattice damage over time.

14. The method of claim 12, wherein said mounting a neutron source adjacent the material specimen comprises mounting the neutron source to the material specimen.

15. The method of claim 14, wherein said mounting a detector adjacent the material specimen comprises mounting the detector to the material specimen.

16. The method of claim 15, further comprising positioning a shield adjacent the neutron source to absorb stray neutrons.

17. The method of claim 16, further comprising positioning a moderator between the neutron source and the material specimen.

18. The method of claim 12, wherein mounting a neutron source adjacent the material specimen comprises mounting an isotopic neutron source adjacent the material specimen.

19. The method of claim 12, wherein continuing to collect and store positron annihilation data is performed while the material specimen is in service.

20. (Canceled).

21. The method of claim 12, further comprising:

retrieving stored positron annihilation data; and

processing the positron annihilation data in accordance with a Doppler-broadening algorithm to produce output data indicative of an accumulation of lattice damage over time.

22. The method of claim 1, further comprising removing the neutron source before collecting positron annihilation data.

23. The method of claim 12, further comprising removing the neutron source before collecting positron annihilation data.

24. (Canceled).

EVIDENCE APPENDIX

None.

RELATED PROCEEDINGS APPENDIX

1. *Ex parte Akers,* Appeal No. 2005-0855 (Bd. Pat. App. & Interf. 2005) (slip op.).

The opinion in support of the decision being entered today was not written for publication and is not binding precedent of the Board.

UNITED STATES PATENT AND TRADEMARK OFFICE

BEFORE THE BOARD OF PATENT APPEALS AND INTERFERENCES

Ex parte DOUGLAS W. AKERS

Appeal No. 2005-0855
Application No. 10/269,807

HEARD: May 18, 2005

Before PATE, MCQUADE, and BAHR, *Administrative Patent Judges*.
MCQUADE, *Administrative Patent Judge*.

DECISION ON APPEAL

Douglas W. Akers originally took this appeal from the final rejection (mailed June 16, 2003) of claims 1 and 8 through 39, all of the claims pending in the application. After the appellant's main and reply briefs (filed October 3, 2003 and January 13, 2004) and an examiner's answer (mailed December 1, 2003) had been made of record, the examiner issued an Office action (mailed February 25, 2004) reopening prosecution and entering superseding rejections of all of the claims. Pursuant to 37 CFR § 1.193(b)(2)(ii), the appellant then submitted a request that the appeal be reinstated (filed April, 14, 2004) and

a supplemental brief (filed August 2, 2004). The examiner, implicitly granting the request, entered a second answer (mailed September 14, 2004) and forwarded the application to this Board for review of the new rejections of claims 1 and 8 through 39.

THE INVENTION

The invention relates to "methods . . . for performing non-destructive testing of materials using positron annihilation" (specification, page 1). Representative claim 1 reads as follows:

1. A method, comprising:
determining whether a specimen to be tested includes at least one positron emitter therein that will be activated in response to photon bombardment;
selecting a positron emitter to be activated;
determining a threshold photon energy required to activate the selected positron emitter;
determining a half-life of the selected positron emitter; and
when the half-life of the selected positron emitter is less than a selected half-life, then performing a rapid activation/analysis process, said rapid activation/analysis process comprising:
activating for an activation time the selected positron emitter by bombarding the specimen with photons having energies at least as great as the threshold photon energy;
detecting for a detection time gamma rays produced by annihilation of positrons with electrons in the specimen; and
repeating said steps of activating for an activation time and detecting for a detection time until detecting a sufficient number of gamma rays to determine at least one material characteristic of said specimen;

when the half-life of the selected positron emitter is greater than or equal to the selected half-life, then performing a normal activation/analysis process, said normal activation/analysis process comprising:

activating the selected positron emitter by bombarding the specimen with photons having energies at least as great as the threshold photon energy; and

detecting gamma rays produced by annihilation of positrons with electrons in the specimen.

THE REJECTIONS

Claims 1 and 8 through 39 stand rejected under 35 U.S.C. § 112, first paragraph, as being based on a specification which fails to comply with the enablement requirement.

Claims 1 and 8 through 39 also stand rejected under 35 U.S.C. § 112, second paragraph, as failing to particularly point out and distinctly claim the subject matter the appellant regards as the invention.

Attention is directed to the main, reply and supplemental briefs and the second answer for the respective positions of the appellant and the examiner regarding the merits of these rejections.[1]

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[1] In the Office action which reopened prosecution, claims 1 and 8 through 10 additionally stood rejected under 35 U.S.C. § 112, first paragraph, as being based on a specification which fails to comply with the written description requirement. Upon reconsideration, the examiner has withdrawn this rejection (see page 2 in the second answer). Presumably, the examiner also has withdrawn any reasoning relating to the two remaining rejections which was set forth in the Office action but not restated in the

(continued...)

DISCUSSION

I. Preliminary matter

In the supplemental brief (see pages 3, 4 and 17) and second answer (see pages 11 and 12), the appellant and the examiner debate the propriety of the Office action which reopened prosecution subsequent to appeal. As this matter is not directly connected with the merits of any issue involving a rejection of claims, it is reviewable by petition to the Director rather than by appeal to this Board (see In re Hengehold, 440 F.2d 1395, 1403-04, 169 USPQ 473, 479 (CCPA 1971), and hence will not be further addressed in this decision.

II. The 35 U.S.C. § 112, first paragraph, rejection

The dispositive issue with respect to the enablement requirement of 35 U.S.C. § 112, first paragraph, is whether the appellant's disclosure, considering the level of ordinary skill in the art as of the date of the application, would have enabled a person of such skill to make and use the claimed invention without undue experimentation. In re Strahilevitz, 668 F.2d 1229, 1232, 212 USPQ 561, 563-64 (CCPA 1982). In calling into

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[1](...continued)
second answer (see Ex parte Emm, 118 USPQ 180, 181 (Bd. App. 1957)).

question the enablement of the disclosure, the examiner has the initial burden of advancing acceptable reasoning inconsistent with enablement. Id.

The examiner considers the appellant's disclosure to be non-enabling in four respects:

> . . . There is neither an adequate description nor enabling disclosure as to what is encompassed by the term, "activating a positron emitter". A "positron emitter" is inherently already activated, i.e., it is radioactive.
>
> At best, the use of the term "activating a positron emitter" is superfluous.
>
> At worst, the term would imply that a positron emitter is either being transformed to another positron emitter or its energy level is further raised by the energy of the activating photon. There is no support in the specification for either one of these two alternatives [second answer, page 3];
>
> There is neither an adequate description nor enabling disclosure as to how and in what manner potential interferences in the data are accounted for in the analysis. For example, Claim 1 recites the step of bombarding the specimen with photons at least as great as the threshold photon energy required to activate the selected positron emitter and detecting gamma rays produced by annihilation of positrons with elections in the specimen.
>
> . . . [T]here is no support as to how one would differentiate between the signals from the selected positron emitter and from the non-selected ones [second answer, pages 6 and 7];
>
> There is neither an adequate description nor enabling disclosure as to how and in what manner one should select an algorithm from a plurality of available algorithms, modify/manipulate the selected algorithm and evaluate the constants in the selected

> algorithm to fit Appellant's situation. Appellant himself admits in the specification that there is not only one known algorithm but rather a plurality of known positron lifetime algorithms (e.g. see paragraph 0058), Doppler broadening algorithms (paragraph 0057) and three-dimensional imaging algorithms (e.g., see paragraph 0060).
>
> . . . There is no support as to how and in what manner one selects the specific algorithm to use for the two activation/analysis processes, to evaluate requisite constants and to modify the selected algorithm to Appellant's situation [second answer, page 7];

and

> There is neither an adequate description nor enabling disclosure as to how and in what manner one can determine when the half-life of the selected positron emitter is less than a selected half-life (*sic*), where the composition of the specimen is unknown and it is this composition that is desired to be determined. The same lack of support exists for the determination of when the half-life of the selected positron emitter is more than a selected half-life (*sic*) [second answer, page 8].

A fair assessment of the appellant's disclosure shows that the references therein to "activating" a positron emitter through photon bombardment of the specimen would be understood by the artisan as synonymous with "producing" or "forming" the positron emitter from a stable precursor. For example, the specification states that "photons 16 from the photon source 12 <u>produce</u> such neutron-deficient isotopes . . . referred to herein in the alternative as 'positron emitters'" (page 7, emphasis added), and

that "one way for generating positrons is through the formation within the specimen 18 of neutron-deficient isotopes, i.e., positron emitters" (page 20, emphasis added). In the same vein, the specification describes Tables I and II (on pages 21 and 22) as identifying "those isotopes that may be converted into positron emitters by photon bombardment" (page 20, emphasis added). Thus, even if the appellant's description of "activating" a positron emitter is somewhat inaccurate as urged by the examiner, it is so only in the most hyper-technical sense. Read in context, the appellant's terminology would not pose any enablement problem from the perspective of a person having ordinary skill in the art.

The examiner's concerns as to possible interference between respective signals produced by the selected positron emitter and non-selected positron emitters and as to the half-life of the selected positron emitter also are unfounded, primarily because they are not commensurate with the scope of the invention disclosed and claimed by the appellant. In this regard, the claims do not exclude the activation of multiple positron emitters, and indeed the appellant's specification (see pages 8, 13 and 14) actually allows for such activation. The claims also

do not require the composition of the specimen to be unknown, and are not directed to a method for determining the composition of the specimen.

Finally, while the appellant's disclosure does not convey much detail as to the various algorithms described therein, these algorithms admittedly are generally known in the art. The examiner has failed to advance any cogent reasoning as to why the disclosure would not have enabled a person having ordinary skill in the art to employ these algorithms, without undue experimentation, to the extent required by the appealed claims.

Hence, the examiner's position that the appellant's disclosure, considering the level of ordinary skill in the art as of the date of the application, would not have enabled a person of such skill to make and use the claimed invention without undue experimentation is not well taken. Therefore, we shall not sustain the standing 35 U.S.C. § 112, first paragraph, rejection of 1 and 8 through 39.

III. The 35 U.S.C. § 112, second paragraph, rejection

The second paragraph of 35 U.S.C. § 112 requires claims to set out and circumscribe a particular area with a reasonable degree of precision and particularity. In re Johnson, 558 F.2d

1008, 1015, 194 USPQ 187, 193 (CCPA 1977). In determining whether this standard is met, the definiteness of the language employed in the claims must be analyzed, not in a vacuum, but always in light of the teachings of the prior art and of the particular application disclosure as it would be interpreted by one possessing the ordinary level of skill in the pertinent art. Id.

The examiner views the appealed claims to be indefinite for reasons essentially similar to those listed above in connection with the enablement rejection. In this regard, the examiner points to the claim limitations relating to (1) the activation of a positron emitter, (2) the positron lifetime, Doppler broadening, three-dimensional imaging and activation/analysis process algorithms and (3) the determination of the half-life of the selected positron emitter (see pages 9 through 11 in the second answer). For the reasons explained previously, the limitations pertaining to the activation of a positron emitter would have been readily understood by the artisan when read in light of the underlying specification. Furthermore, the examiner's criticisms of the claim limitations pertaining to the algorithms and the half-life of the selected positron emitter

focus on the breadth of these limitations. It is well settled, however, that mere breadth does not equate to indefiniteness. In re Miller, 441 F.2d 689, 169 USPQ 597, 600 (CCPA 1971). Accordingly, the examiner's contention that the appealed claims are indefinite is unpersuasive.

Thus, we shall not sustain the standing 35 U.S.C. § 112, second paragraph, rejection of claims 1 and 8 through 39.

SUMMARY

The decision of the examiner to reject claims 1 and 8 through 39 is reversed.

REVERSED

WILLIAM F. PATE, III Administrative Patent Judge	
JOHN P. MCQUADE Administrative Patent Judge	BOARD OF PATENT APPEALS AND INTERFERENCES
JENNIFER D. BAHR Administrative Patent Judge	

JPM/kis

ALAN D. KIRSCH
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REFERENCES APPENDIX

Copies of the following references are attached hereto for the Board's convenience:

1. U.S. Patent No. 4,064,438 issued to Alex, et al.

2. U.S. Patent No. 6,178,218, issued to Akers, et al.

3. U.S. Patent No. 7,058,153, issued to Akers.

4. Y. Zhu & R. Gregory, "Analysis of Positron Annihilation Lifetime Data Presented as a Sum of Convoluted Exponentials with the Program "SPLMOD," *Nuclear Instruments & Methods in Physics Research A284*, 443-451 (1989).

5. J. Schaffer, "Deconvoluted Doppler Broadened Positron Annihilation Spectroscopy: Characterization of Defects in Aluminum," Ph.D. Thesis, Duke University, University Microfilms International (1985).

6. P. Derlet, T. Choy, "A positron annihilation lifetime spectroscopy study of porous silicon using a continuous lifetime fitting algorithm," *Journal of Material Science Letters 15*, 1949-1952 (1996).

7. P. Bandžuch, M. Morháč, J. Krištiak, "Study of Van Cittert and Gold iterative methods of deconvolution and their application in the deconvolution of experimental spectra of positron annihilation," *Nuclear Instruments & Methods in Physics Research A384*, 506-515 (1997).

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Nuclear Instruments and Methods in Physics Research A284 (1989) 443–451
North-Holland, Amsterdam

ANALYSIS OF POSITRON ANNIHILATION LIFETIME DATA PRESENTED AS A SUM OF CONVOLUTED EXPONENTIALS WITH THE PROGRAM "SPLMOD"

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Received 12 December 1988 and in revised form 12 June 1989

The reliability of a least squares analysis of positron annihilation lifetime data represented as a sum of convoluted exponentials is investigated with computer-stimulated test data. The method of analysis, which is available as a computer program called "SPLMOD" [R.H. Vogel, Technical Report EMBL-DA08, European Molecular Biology Laboratory, Heidelberg, FRG, (1986)], avoids direct determination of the instrument resolution function by employing the decay curve of a reference material with a well-known single lifetime. The performance of the algorithm for extracting positron annihilation lifetime information was evaluated by using several measures of the information content of the decay curve described recently by Schrader and Usmar [in: Positron Annihilation Studies of Fluids, ed. S. Sharma (World Scientific, Singapore, 1988)]. The sensitivity of the algorithm to systematic errors including errors in the resolution function, shifts in the zero time channel and contamination of the reference decay curves by additional lifetime components was evaluated. The method provides excellent estimates of lifetime parameters when the reference decay curve accurately reflects the resolution function of the sample data. However, the algorithm is extremely sensitive to errors in the instrument resolution function.

1. Introduction

The analysis of positron annihilation lifetime data is an extremely difficult undertaking. The decay curve is usually represented by:

$$C(t) = \sum_{i=1}^{n} \alpha_i \lambda_i \exp(-\lambda_i t), \tag{1}$$

where α_i is the number of positrons annihilating with natural lifetime, λ_i^{-1}. Analysis of sums of exponentials is notoriously difficult, particularly when the number of components, n, is unknown. In general, even for data with arbitrarily small noise levels, there exist a large number of solutions, $[\alpha_i, \lambda_i, n]$, that fit the data to within the noise level. These difficulties are compounded by the fact that in a positron annihilation lifetime experiment one cannot observe the function $C(t)$ directly, only its convolution with the instrument resolution function, $R(t)$:

$$y(t) = R(t) * C(t). \tag{2}$$

The difficulties associated with the analysis of eq. (2) are therefore two-fold: the choice of an appropriate representation of $C(t)$ and the determination of the function, $R(t)$.

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The problems associated with analysis of data with eq. (1) are very well known. In general, we have no prior knowledge of the number of components, n, in eq. (1). If n is too large the solutions become very unstable to noise in the data. Because of this difficulty, it is common to assume only two or three components in eq. (1). This has the effect of stabilizing the solution to noise and in some simple systems may provide a physically meaningful representation of the decay. However, in more complex systems setting n too small will result in an inadequate representation of the system, resulting in a loss of valuable information and a set of α_i and λ_i pairs that may have little or no physical meaning. Because of the non-linearity of $C(t)$ in the λ_i, it is not possible to extend linear hypothesis tests to define an upper value for n. However, Provencher [1] has described a hypothesis test which incorporates a correction for non-linearity that has been found to be very effective. It is employed in the programs DISCRETE, which solves sums of exponentials and SPLMOD which solves more general sums of one parameter functions, including exponentials and convoluted exponentials. The use of eq. (1) assumes that a discrete sum of exponentials is a physically meaningful representation of the data. For many simple, homogeneous systems this is

indeed the case, however, for complex, heterogeneous systems and systems in which distinct structural domains persist for times that are long relative to positron lifetimes, the lifetimes spectrum is expected to be more complex and may consist of a continuous distribution of lifetimes over some interval. For such systems an alternative approach is to replace the sum in eq. (1) by an integral [2–4]:

$$C(t) = \int_0^\infty \lambda\alpha(\lambda) \exp(-\lambda t)\, d\lambda = \mathscr{L}\{\lambda\alpha(\lambda)\}. \quad (3)$$

$C(t)$ is simply the Laplace transform of $\lambda\alpha(\lambda)$, where $\alpha(\lambda)$ is the annihilation rate probability density function (pdf). The fraction of positrons annihilating with rates between λ and $\lambda + d\lambda$ is then given by $\alpha(\lambda)\, d\lambda$ (assuming $\alpha(\lambda)$ is appropriately normalized). In principle, $\alpha(\lambda)$ can be recovered by inverse Laplace transformation of $C(t)$. The problems of solution uniqueness and stability to noise associated with analysis of eq. (1) also plague the inversion of eq. (3). However, recent advances in the solution of Fredholm integral equations provide a number of reliable inversion methods [4–9].

Schrader [2,3] has pioneered the application of Laplace transform methods in the analysis of positron annihilation lifetime data and the application of information theory approaches to the determination of the information content of the experimental data. A particularly important result of this work is the expression of the information content (Shannon Number) of the data in terms of spectrometer parameters (i.e. the number of channels, the channel width, FWHM and the total number of annihilation events observed). Not only does this knowledge define the complexity of the function, $C(t)$, that is required to properly represent the data, but it also serves as a guide in the design of experiments to maximize the information content of the data.

The accurate determination of the instrument resolution function, $R(t)$, is a major problem in analysis of positron lifetime data. Probably the most widely used method is to determine $R(t)$ from the prompt spectrum of a ^{60}Co source. However, the resolution function is very dependent on the distribution of energy deposited in the scintillators. As a result, the function determined with the 1.17 MeV and 1.33 MeV coincident γ-rays from ^{60}Co will not correctly represent the resolution function when data are collected with a ^{22}Na source. One approach, that attempts to overcome these difficulties, is to determine the resolution function from the lifetime data themselves. An analytical function, such as a sum of Gaussians or a modified Gaussian, is assumed for $R(t)$ and its parameters are treated as variables to be determined along with the lifetime parameters of interest [10,11]. However, there are several fundamental objections to this approach. The addition of further parameters to be determined by the analysis can severely compound the problem of solution uniqueness. In addition, the approach requires the choice of an analytical function to represent the resolution properties of the instrument. An incorrect choice will, of course, transmit errors to the lifetime estimates.

The resolution function may also be determined in a separate experiment from the decay curve of a standard sample with a known single lifetime, such as a well-annealed metal [12]. In principle, this method can yield very good estimates of the instrument resolution function. However, in practice, annihilation in the source and positron trapping at the surface can give rise to additional components. An alternative approach is to employ a ^{207}Bi source. ^{207}Bi emits two γ-rays separated by a time interval of 186 ps, the energies of which are almost identical to those employed in a positron lifetime experiment with a ^{22}Na source. Although the method does not introduce unwanted source components, it is not yet clear if the energies of the γ-rays emitted by ^{207}Bi are sufficiently similar to those occurring with ^{22}Na that the types of error associated with the use of ^{60}Co are entirely avoided.

At present, the use of standard samples with ^{22}Na sources appears to offer the best hope for reliable determination of the instrument resolution function. We have been interested in the use of a deconvolution method due to Gauduchon and Wahl [13] and Wijnaendts van Resandt et al. [14] for this purpose. A preliminary report of its use in the analysis of positron annihilation lifetime data with numerical Laplace inversion methods has appeared [4] but no tests of its performance have been presented. Our purpose in this paper is to explore the reliability of this deconvolution method in the analysis of positron annihilation lifetime data. The efficiency of the algorithm for extracting lifetime information is evaluated by using several measures of the information content of the decay curve described by Schrader and Usmar [3]. In this work, $C(t)$ is represented by a sum of exponential terms as in eq. (1) and the analysis is performed with the FORTRAN program, SPLMOD, developed by Vogel [15]. Although eq. (1) is more restrictive than eq. (3), it can be a valid representation of annihilation lifetimes in simple, homogeneous systems and is considerably simpler for our purpose because the measure of information content of the data, the Shannon Number, is directly related to the number of components in the lifetime spectrum.

2. Deconvolution of the instrument resolution function

Deconvolution of the instrument resolution function follows the method of Gauduchon and Wahl [13] and Wijnaendts van Resandt et al. [14], which avoids the direct determination of $R(t)$ by measuring, $y_r(t)$, the

decay curve of a reference material with a well-known single lifetime, λ_r:

$$y_r(t) = R(t) * C_r(t), \tag{4}$$

where

$$C_r(t) = \alpha_r \lambda_r \exp(-\lambda_r t). \tag{5}$$

Convoluting eq. (2) with $C_r(t)$ we obtain:

$$C_r(t) * y(t) = y_r(t) * C(t). \tag{6}$$

Here we assume that $y_r(t)$ and $y(t)$ have the same resolution function, $R(t)$. This would be true if the reference and sample decay curves could be measured simultaneously, but this is not possible in a positron annihilation lifetime experiment. Any instrument drift occurring between measurement of the sample and reference decay curves will therefore introduce error into the lifetime estimates. This, of course, is true of all methods that involve a separate measurement of the resolution function of the instrument and can only be avoided by improving the stability of the instrument.

Eq. (6) can be rewritten as:

$$\alpha_r \lambda_r \{\exp(-\lambda_r t)\} * y(t) = y_r(t) * C(t), \tag{7}$$

which on taking Laplace transforms gives:

$$\frac{\alpha_r \lambda_r}{\lambda_r + p} \tilde{y}(p) = \tilde{y}_r(p) \tilde{C}(p), \tag{8}$$

where the tilde denotes Laplace transformation and p is the Laplace variable. Eq. (8) is solved for $\tilde{y}(p)$:

$$\tilde{y}(p) = \alpha_r^{-1} \lambda_r^{-1} \{\lambda_r \tilde{y}_r(p) \tilde{C}(p) + p \tilde{y}_r(p) \tilde{C}(p)\}, \tag{9}$$

which on inverting Laplace transforms gives:

$$y(t) = \alpha_r^{-1} \lambda_r^{-1} \{\lambda_r y_r(t) * C(t) + y_r(t) * [C'(t) + C(0)\delta(t)]\}. \tag{10}$$

If $C(t)$ is represented by eq. (1), eq. (10) becomes:

$$y(t) = \sum_{i=1}^{n} \frac{\alpha_i \lambda_i}{\alpha_r \lambda_r} \{ y_r(t) + (\lambda_r - \lambda_i) y_r(t) * \exp(-\lambda_i t)\}. \tag{11}$$

If λ_r is known and α_r is absorbed into the α_i, eq. (11) must be solved for the $2n$ parameters α_i and λ_i. If λ_r is not known, there are $2n+1$ parameters.

3. Analysis of sums of convoluted exponentials with "SPLMOD"

SPLMOD analyzes data that can be represented as a sum of one parameter functions:

$$y_k = \sum_{i=1}^{n} \beta_i f(\lambda_i, t_k) + \sum_{i=1}^{n_L} \gamma_i g_i(t_k). \tag{12}$$

The current version of SPLMOD (version 3) distributed by Vogel [15] can perform the following types of analysis of relevance to Positron Annihilation Lifetime (PAL) spectroscopy:

(a) Solution of eq. (12) when the resolution function is known; i.e. with $f(\lambda_i, t_k) = R(t_k) * \exp(-\lambda_i t_k)$ and $g_1(t_k) = 1$ (to account for the background).

(b) Solution of eq. (12) using a reference material with a known single annihilation lifetime, λ_r, i.e. with $f(\lambda_i, t_k) = (\lambda_r - \lambda_i) y_r(t_k) * \exp(-\lambda_i t + y_r(t_k))$ and $g_1(t_k) = 1$.

(c) Solution of eq. (12) using a reference material with a single annihilation lifetime which need not be known; i.e. with $f(\lambda_i, t_k) = y_r(t_k) * \exp(-\lambda_i t_k)$, $g_1(t_k) = 1$ and $g_2(t_k) = y_r(t_k)$.

We have employed option (b) in our simulations because it provides more stable solutions than option (c).

SPLMOD performs a weighted least squares analysis in which $f(\lambda_i, t_k)$ is approximated by a sum of normalized cubic B-splines. The program employs Gauss–Newton minimization, with an extensive search of parameter space to determine the initial parameter values. The convolution, $y_r(t_k) * \exp(-\lambda_i t)$, is calculated by using a recursive formula of Grinvald and Steinberg [16]:

$$f(\lambda_i, t_{k+1}) = \{f(\lambda_i, t_k) + 0.5\Delta t y_r(t_k)\} \times \exp(-\lambda_i \Delta t) + 0.5\Delta t y_r(t_{k+1}), \tag{13}$$

where Δt is the channel width of the multi-channel analyzer in which the data are collected. SPLMOD performs several analyses in which n in eq. (1) takes the values: 1, 2, 3,... n_{max}, where n_{max} is set by the user. SPLMOD supplies a number of statistical measures, including Fisher probabilities and random runs probabilities, to aid in the choice of an appropriate solution. Measures of the information content of the data may also be employed to define an appropriate solution [3].

Note that it is not necessary to independently define the zero time point of the spectrometer. This information is already contained in the reference decay curve. However, there is an option in SPLMOD to correct for small changes in the zero time point due to instrument drift occurring between measurement of sample and reference decay curves.

4. Simulation of decay curves

Positron annihilation decay curves have been simulated by convoluting eq. (1) with a Gaussian resolution function with FWHM equal to $2\sigma\sqrt{\ln 2}$:

$$R(t) = \frac{1}{\sigma\sqrt{\pi}} \exp -(t/\sigma)^2. \tag{14}$$

This convolution is given by:

$$y(t) = 0.5 \sum_{i=1}^{n} \alpha_i \lambda_i \exp\left\{ -\lambda_i t + (\lambda_i \sigma/2)^2 \right\} \times \operatorname{erfc}(\lambda_i \sigma/2 - t/\sigma). \tag{15}$$

where erfc is the compliment of the error function:

$$\operatorname{erfc}(x) = 1 - \operatorname{erf}(x) = 1 - \frac{2}{\sqrt{\pi}} \int_0^x \exp(-t^2)\, dt. \tag{16}$$

Conversion of the continuous function, $y(t)$, to a table of channel counts, y_k, was performed by numerical integration. A background and appropriate Poisson noise were added to each channel. The reference data were simulated in the same way except that no background was added. The reference and sample spectra were calculated over the same range of channels in each case.

5. Information content of the simulated data

Schrader and Usmar [3] have given a detailed discussion of the determination of the information content (Shannon Number) of decay curves and have provided an approximate expression for the Shannon Number in terms of instrument setting of the spectrometer. The Shannon number, in the context of PAL spectroscopy, is a measure of the number of resolvable lifetimes that can be geometrically fitted between the largest and smallest resolvable lifetimes. This measure is an approximation because it depends on ones definition of the relative scatter in the decay curve and on the values that are chosen for the largest and smallest resolvable lifetimes. Schrader and Usmar [3] define the Shannon Number, F, as:

$$F = \pi^{-1} \omega_{max} \ln(a_1 N_{ch} \Delta t / a_2 \text{ FWHM}), \tag{17}$$

where a_1 and a_2 are constants, FWHM is the full width at half the peak height of the resolution function, N_{ch} is the number of channels to the right of the zero-time channel, N_0, employed in the analysis (a maximum value for N_{ch} is defined by the number of channels for which the count is greater than the square-root of the background count) and ω_{max} is defined by:

$$\omega_{max} = 2\pi^{-1} \ln(\sqrt{2\pi}/\eta), \tag{18}$$

η is a measure of the effective relative noise in the decay curve and is defined as:

$$\eta = \sum_{k=N_0}^{N_{ch}} y_k^{1/2} \Big/ \sum_{k=N_0}^{N_{ch}} y_k, \tag{19}$$

ω_{max} has a special significance in the eigenfunction expansion of Laplace transforms which we need not be concerned with here [3,5]. Eq. (18) is derived by assuming that the shortest resolvable lifetime is equal to a_2FWHM and the longest resolvable lifetime is equal to $a_1 N_{ch} \Delta t$. A resolution factor, p, is defined as the ratio of resolvable lifetimes and it follows that F is the number of resolvable lifetimes that can be geometrically fitted between a_2FWHM and $a_1 N_{ch} \Delta t$. The constants a_1 and a_2 need to be determined. In practice, the shortest resolvable lifetime is probably less than FWHM and the longest resolvable lifetime is longer than $N_{ch} \Delta t$, so $a_2 < 1$ and $a_1 > 1$. Schrader and Usmar [3] suggest $a_1 = 3$ and $a_2 = \frac{1}{3}$ as reasonable values when a_2FWHM $> 3\Delta t$, but they suggest replacing a_2FWHM by $3\Delta t$ if a_2FWHM $< 3\Delta t$.

The resolution factor is given by:

$$p = \exp(\pi/\omega_{max}) \tag{20}$$

and is therefore dependent on the definition of the effective relative noise of the decay curve (eq. (19)). Estimates of a_1, a_2 and the correctness of eq. (19) are discussed below.

6. Analysis of simulated data

Table 1 lists the results of an analysis of simulated PAL data together with the information parameters for the decay curve and will serve as a point of reference for our subsequent discussions. The simulated data contain three components. The reference has a single lifetime of 125 ps. A total of 800 channels were analyzed, starting 30 channels (0.75 ns) to the left of the peak. A plot of

Table 1
Calculated information content of simulated data and results of its analysis with SPLMOD

FWHM	290 ps	p	2.6
Δt	25 ps	η	0.015
Reference lifetime	125 ps	ω_{max}	3.25
Total events	10^6	maximum N_{ch}	442

a_1	a_2	F	Resolvable lifetimes (ns)	
			min.	max.
1	1	3.8	0.29	11
2	0.5	5.2	0.15	22
3	0.33	6.0	0.1	33

		Lifetimes (ns)	
Simulated	0.125	0.400	2.000
Fitted	0.124	0.397	1.997
		Alpha	
Simulated	0.130	0.470	0.400
Fitted	0.125	0.474	0.401
		Background	
Simulated		100	
Fitted		100.5	

($a_2 = 0.25$ to 0.20). Beyond this value, SPLMOD is still able to identify three components but the parameter values become very poor. Increasing the total count to 10^7 does not improve these estimates. At a FWHM of 290 ps, a value that is typical of modern PAL spectrometers employing plastic scintillators, the shortest lifetime that can be resolved by SPLMOD is approximately 50 ps (i.e. $a_2 = 0.17$). An estimate of a_1 was determined by varying the number of channels employed in the analysis. In all cases the start channel was sufficiently far to the left of the peak (−0.74 ns) to sample the baseline. With $N_{ch} = 1940$, the longest lifetime that can be resolved is approximately 100 ns ($a_1 = 4$).

We have examined the ability of the program to resolve lifetime components and were particularly inter-

Table 3
The resolution of lifetime components with SPLMOD. Variations in the effective relative noise and resolution factor were generated by changing the total number of events. Simulation parameters were; FWHM = 290 ps, $\Delta t = 12.5$, reference lifetime = 125 ps and background = 100

		Simulated	Fitted	Fitted	Fitted
Total events			10^6	10^5	10^4
Relative noise			0.024	0.054	0.074
ω_{max}			3.0	2.4	2.4
Resolution factor			2.9	3.6	4.1
$F(a_1 = 4, a_2 = 0.25)$			6.1	4.5	2.7
Maximum N_{ch}			959	451	64
Lifetime	1	0.125	0.122	0.113	0.124
(ns)	2	0.400	0.386	0.313	0.609
	3	1.280	1.213	0.895	2.786
	4	4.096	3.947	3.338	–
Alpha	1	0.250	0.245	0.223	0.341
	2	0.250	0.247	0.210	0.345
	3	0.250	0.248	0.258	0.314
	4	0.250	0.260	0.310	–

Table 4
The effect of systematic errors on lifetime parameters estimated by SPLMOD. Simulation parameters were FWHM = 290 ps, $\Delta t = 12.5$ ps, background = 100, total events = 10^7 and reference lifetime = 125 ps

		Simulated data	Incorrect reference FWHM		Zero channel shift
			285 ps	295 ps	
Lifetime	1	0.125	0.127	0.138	0.134
(ns)	2	0.400	0.409	0.410	0.409
	3	2.000	2.004	2.004	2.005
	4	–	0.003	100.0	0.002
Alpha	1	0.130	0.663	0.148	0.247
	2	0.470	0.171	0.449	0.402
	3	0.400	0.150	0.395	0.351
	4	–	0.016	0.008	0.001
Background		100	100.4	91.1	99.9

		Simulated data	Contamination of reference by additional component with lifetime = 450 ps		
Contaminant %			5	10	15
Lifetime	1	0.125	0.122	0.120	0.118
(ns)	2	0.400	0.382	0.365	0.347
	3	2.000	2.001	2.003	2.005
Alpha	1	0.130	0.131	0.135	0.137
	2	0.470	0.476	0.474	0.477
	3	0.400	0.393	0.391	0.386
Background		100	100.3	100.2	100.1

ested in determining if the value of the resolution factor calculated according to eq. (20) correctly predicted the point at which SPLMOD failed to resolve lifetime components. An example of the results for such a test is shown in table 3. The simulated data consisted of four components with successive lifetimes increasing by a factor of 3.2. When the total number of events is 10^6, the calculated resolution factor is 2.9 and the Shannon number, F, is 6.1 SPLMOD is able to resolve the four components and provides reasonably good estimates of the lifetime parameters. When the total number of events is reduced to 10^5, the effective relative noise is doubled, the resolution factor increases to 3.6 and the Shannon number decreases to 4.5. SPLMOD is still able to resolve four components but the lifetime parameter values become poor. When the total number of events is reduced to 10^4, the relative noise increases to 0.074, the resolution factor increases to 4.1 and the Shannon Number decreases to 2.7. SPLMOD is unable to resolve the four components. Eq. (19) thus appears to provide a good estimate of the effective relative noise in the data as measured by the predictive power of the calculated resolution factor.

7. Systematic errors

We have examined the sensitivity of the SPLMOD algorithm to various systematic errors in the data. The most important sources of systematic error arise from: (i) variations in the resolution function for the reference and sample data, (ii) differences in the zero time point for the reference and sample, and (iii) contamination of the reference with additional lifetime components.

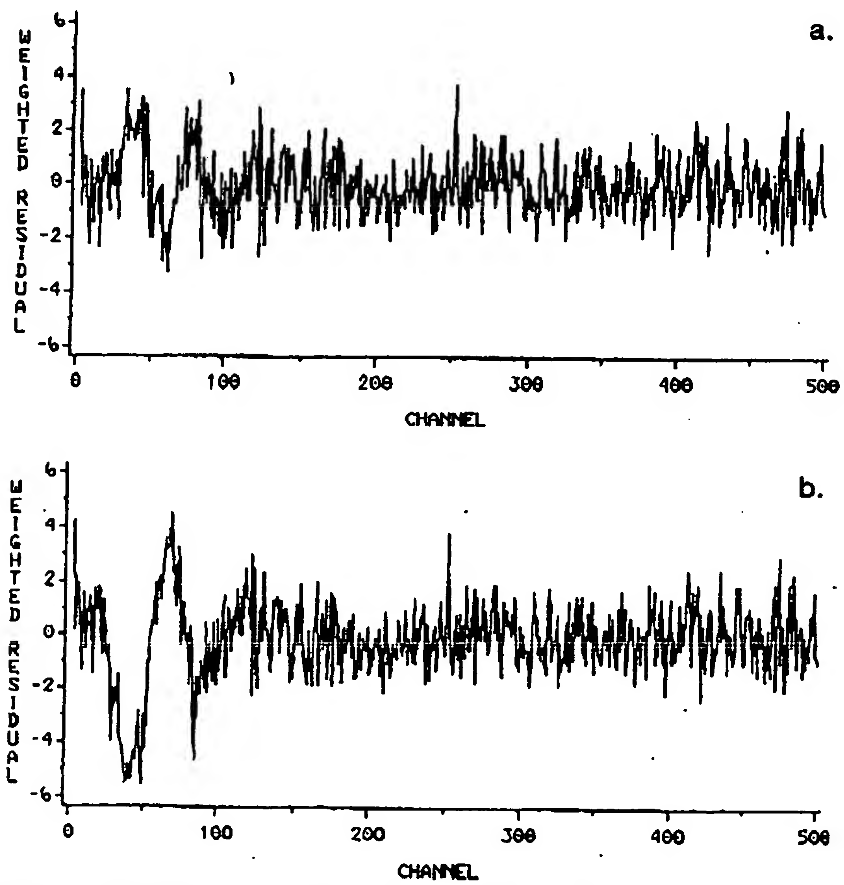

Fig. 2. Effect of errors in the FWHM of the reference decay curve on the weighted residuals. The lifetime parameters are listed in table 4. The FWHM of the simulated sample decay curve was 290 ps. Sample data was analyzed using reference decay curves with FWHM of (a) 285 ps and (b) 295 ps.

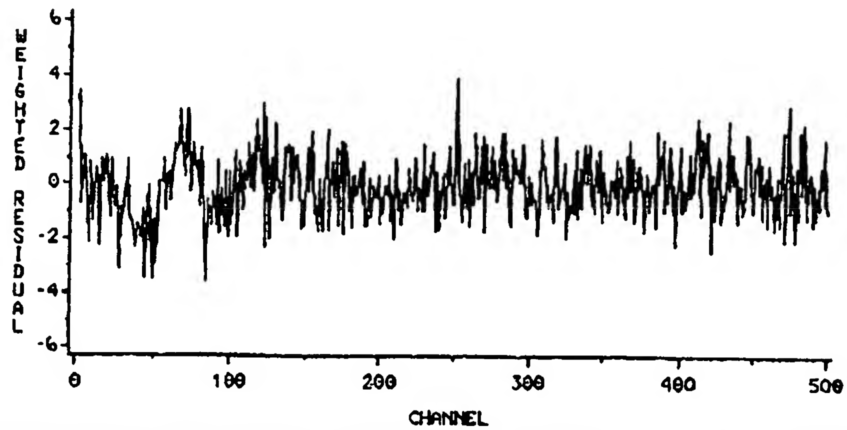

Fig. 3. Effect of a shift in the zero time channel on the weighted residuals. The lifetime parameters are listed in table 4. The reference decay curve was shifted by −2.5 ps with respect to the sample decay curve.

The fitted lifetime parameters are extremely sensitive to variations in the FWHM of the resolution function. The lifetime parameters obtained from an analysis of a three component sample (FWHM = 290 ps) with reference decays having incorrect FWHM values (285 and 295 ps) are given in table 4. The lifetime parameters determined by SPLMOD when the FWHM for the reference is less than that employed for the sample are very poor. The intensities of all components are grossly in error. In addition, a spurious short-lived component appears. When the FWHM of the reference is made larger than that employed for the sample, a spurious long-lived component appears (100 ns). Estimates of the other lifetime parameters are in error, but are not nearly as poor as those determined with the smaller reference FWHM. Plots of the residuals are shown in fig. 2. The fits to the data are poor about the peak.

A shift in the zero channel of the reference with respect to the sample data also generates poor estimates of the lifetime parameters and an additional spurious short-lived component. The example given in table 4 and fig. 3 was obtained by shifting the reference decay curve by −2.5 ps with respect to the sample decay curve. This shift is a fifth of the channel width employed. SPLMOD can correct for small shifts in the zero time channel by assuming that $y(t+\epsilon)$ has been used instead of $y(t)$ and then expanding eq. (11) in a Taylor series about $y(t)$ to the first order term. This gives an additional linear term in eq. (12). However, in this case the correction did little to improve the fit to the data.

The analysis assumes the reference to have a single lifetime component, an ideal which is unlikely to be exact for real systems. Annihilation in the source and trapping at the surface of the reference material undoubtedly introduce additional lifetime components. The effect of introducing an additional component with a lifetime of 450 ps into the reference decay curve is shown in table 4. The estimated lifetime parameters are relatively insensitive to the presence of the contaminant, even when it represents 15% of the reference decay. The largest error appears in the sample component which has a lifetime closest to the contaminant lifetime.

8. Conclusions

The results presented in the previous sections suggest that the deconvolution and least squares analysis methods employed by SPLMOD can provide excellent estimates of positron annihilation lifetime parameters for systems that can be represented by a discrete sum of exponentials. As we have mentioned, this representation is too restrictive for many systems of interest in which distributions of positron lifetimes are expected. For such systems numerical Laplace inversion methods are obviously to be preferred. The results of our tests of a modified version of the program, CONTIN [3,5,6], which solves integral equations with convoluted kernels will be published shortly. It is nevertheless clear from the present work, that estimates of the lifetime parameters are critically dependent on accurate knowledge of the instrument resolution function. We doubt that the deconvolution method employed here is any more sensitive to errors in the resolution function than other algorithms that have been described in the literature or that are currently in use. For example, lifetimes reported using ^{60}Co prompt spectra to measure the instrument resolution function are undoubtedly in error since it is known that this method provides a poor estimate of the true resolution function occurring with ^{22}Na sources [3]. There is little doubt that these problems will become

even more severe as we attempt to determine continuous lifetime distributions with numerical Laplace inversion techniques.

Acknowledgements

We are grateful to Dr. Robert Vogel for making a copy of SPLMOD available. This work was supported by grants from the National Science Foundation (DMB 85-18941), Research Corporation (10660), Kent State University Foundation and the National Institutes of Health Biomedical Research Support Grant.

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JOURNAL OF MATERIALS SCIENCE LETTERS 15 (1996) 1949–1952

A positron annihilation lifetime spectroscopy study of porous silicon using a continuous lifetime fitting algorithm

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Porous silicon is a highly complex system containing disorder that exists over a range of scales. Depending on the anodization current and time, and the dopant level and type, the resulting porous layer can have a porosity of up to 80% with a unidirectional columnar-like structure for p^- silicon wafers [1]. The remaining silicon varies in size with characteristic lengths ranging between from 3–4 to 15–30 nm. Such small crystalline structures have an enlarged bandgap due to the quantum confinement effect. The role of confinement in the observed increase in radiative inter-band transition efficiency is however still unclear. How the broken silicon bonds are terminated can directly affect the nature of the inter-band transitions. For example, hydrogen passivation "sweeps" the dangling bond states out of the band gap region; reducing the available non-radiative recombination paths and thereby increasing the efficiency of the radiative transitions. This, however, is not the complete picture since the oxygen content of the porous region has been found in some cases to amplify and change the photoluminescence properties [2]. The electro-chemical processes occurring on the surface during anodization are not yet clearly understood and further experimental characterization is needed.

Positron annihilation lifetime spectroscopy (PALS) provides a unique non-destructive probe into the disorder inherent in porous silicon on the microscopic scale, through the identification of impurity concentrations and types; and on the mesoscopic scale at which the bulk of the porosity exists through the study of positronium lifetimes. Itoh *et al.* [3, 4] and Dannefaer *et al.* [5] have done such an investigation using a discrete lifetime analysis. Itoh *et al.* obtained a satisfactory three-component fit, finding a bulk silicon component (at 230 ps), a defect component (at 600 ps), which they interpreted as arising from either silicon mono-vacancies and/or oxygen divacancies within an $Si-O_2$ layer [6], and a longer 25 ns lifetime due to ortho-positronium annihilating in the porous region. Dannefaer *et al.*, on the other hand, determined that a five-component fit was better, with additional lifetimes arising from para-positronium (at 125 ps) and another ortho-positronium component at 2.5 ns. They attributed the latter to ortho-postronium annihilating in larger vacancy defects either within the remaining silicon or the oxide layer. In this letter we report on a PALS investigation of porous silicon using a continuous lifetime fitting algorithm.

Our motivation lies in the underlying disadvantage in discrete lifetime fitting algorithms where the number of components must initially be assumed since in general a realistic spectrum does not uniquely determine this number. This becomes particularly apparent when looking at highly disordered systems where, indeed, the notion of a discrete spectrum may be invalid. These problems can in part be overcome by using a continuous lifetime fitting algorithm; for example, performing an inverse Laplace transform on the lifetime spectrum, thereby obtaining a probability density function of characteristic lifetimes. The Fortran program CONTIN [7–9] is such an algorithm. Admittedly, use of the inverse Laplace transform does not take into account the instrument resolution function of the apparatus. For the determination of sub-nanosecond lifetimes this entails a distinct loss of accuracy. For well-separated lifetimes that are significantly larger than the typical full width at half maximum (FWHM) of the equipment, the effect is reduced and overshadowed by the loss of accuracy due to the worsening statistics typical for these components. To date, our work appears to be the only systematic study of porous silicon using a continuous lifetime fitting algorithm. This is the first step towards achieving the goal of determining intrinsic lifetime distribution widths for positrons annihilating within the porous silicon layer, and thus its electronic structure.

For the measurement of the annihilation lifetime spectra of porous silicon we employed a standard PALS rig at 200 ps per channel. Such a large timing window is needed to ensure that all lifetime components decay completely into the background. The positron source was $^{22}NaCl$ evaporated onto a 6 μm thick titanium film. Using our PALS rig at 50 ps per channel and the discrete lifetime fitting program PFPOSFIT [10], we obtained for bulk silicon, 221 ± 1 ps at $97 \pm 1\%$ concentration, with a source component lifetime of approximately 429 ± 25 ps at $3 \pm 1\%$ concentration (the iterated instrument resolution had an FWHM of 240 ps with long and short time tails of 50 and 20 ps, respectively.

The porous silicon samples for this investigation were made from 200 μm p^- doped wafers, anodized for 30 min at 20 mA cm^{-2}. The electrolyte used was a 35% ethanoic solution of HF. Under illumination by an ultraviolet (UV) lamp this sample glowed a deep red. The initial thickness of the porous layer

was approximately 50–60 μm. A high resolution scanning electron microscopy (SEM) analysis performed approximately 6 months after the PALS experiment revealed a layer that was approximately 10 μm thick, indicating that structural damage had occurred (Fig. 1). The sample nevertheless still glowed red at a reduced intensity. Fig. 1 reveals the large-scale columnar structure typical of p^- doped porous silicon samples; the remaining (porous) silicon constituting the much thinner connecting membranes between the micrometre-sized pores.

All PALS runs were taken at room temperature (24 °C) in an environment where the temperature could be held constant to within a degree. For each sample, a varying number of spectra were taken (see Table I and Fig. 2), each of which had a maximum peak height of 10^6 counts. Statistical analysis *across* the spectra for a particular sample indicated that to within the noise level, there was no detectable difference between individual runs, justifying the use of the mean spectrum in the analysis using CONTIN. The associated information content analyses [11, 12] are also given in Table I. Here, the Shannon number indicates that in principle up to eight distinct lifetime peaks are resolvable, and the resolution factor suggests that the minimum ratio between these resolvable lifetimes ranges between 2 and 3.

Since CONTIN assumes a spectrum constructed from exponentials, we must choose an appropriate zero-time channel from which the analysis can begin. This must be just beyond the peak of the spectrum, yet not too close to include the "rounding off" effect of the finite instrument resolution. The resulting inverse Laplace transform found by CONTIN is not very sensitive to the choice of the zero-time channel as far as determining distinct components. It is, however, sensitive to determining their intensity, since a shift δt in the zero-time channel will affect the intensity of a component τ by the approximate factor $\exp(-\delta t/\tau)$.

Such an analysis for the 200 ps per channel bulk silicon wafer spectrum is displayed in Fig. 2 for two different zero-time channels; approximately 400 ps (solution 1) and 800 ps (solution 2) beyond the instrumental zero-time channel. Solution 1 contains a dominant broad component centred at approximately 220 ps, which can be attributed to the bulk silicon component. Two long time components can be seen, occurring at approximately 1.5 and 45 ns, the shorter of which can be associated with the common ortho-positronium "pick off" signal present in semiconductors [13]. The extra long 45 ns component does not seem to have been encountered in the literature. We do not know at this stage the origin of this lifetime peak; however, as we shall see, it also appears in the porous silicon sample at an increased intensity. In solution 2, the bulk silicon component becomes broader and less intense, the ratio of its peak height with that of solution 1 being approximately $\exp(\delta t/220)$ where $\delta t \approx 400$ ps. The ortho-positronium peaks at 1.5 and 50 ns acquire more dominance, with their peak heights largely unchanged from solution 1. In addition, we observed a shorter, approximately 125 ps, component, which is most likely to be the accompanying para-positronium signal. That this was not resolved in solution 1 suggests that the "rounding off" effect was not completely removed at 400 ps beyond the approximate zero-time channel.

Fig. 3 displays the CONTIN solution for the porous silicon spectra. Again, solution 1 and solution 2 are for time shifts of approximately 400 and

Figure 1 High resolution SEM picture of the porous silicon sample used in the PALS investigation.

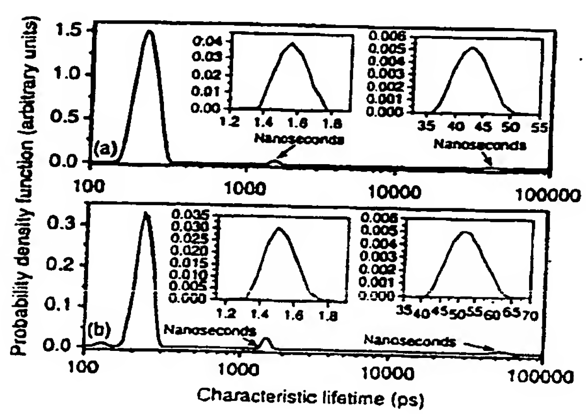

Figure 2 PALS lifetime spectra of (a) bulk silicon and (b) porous silicon taken at 200 ps per channel.

TABLE I The number of PALS spectra taken and the resulting resolution factor and Shannon number

Sample	Number of spectra	Resolution factor	Shannon number
Bulk silicon at 200 ps per channel	49	2	9
Porous silicon at 200 ps per channel	24	3	8

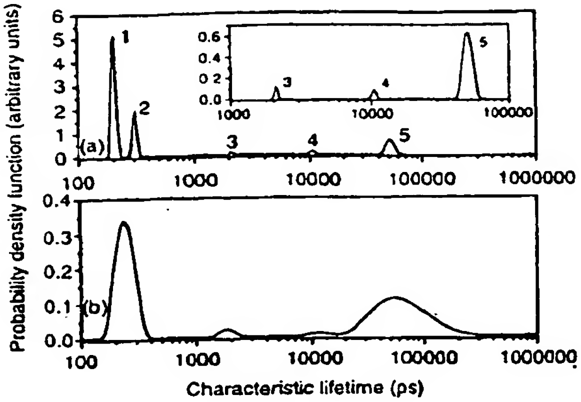

Figure 3 Characteristic lifetime probability density determined using CONTIN for the bulk silicon sample taken at 200 ps per channel. (a) Solution 1: zero-time approximately 400 ps beyond the instrumental zero-time channel. (b) Solution 2: zero-time approximately 800 ps beyond the instrumental zero-time channel.

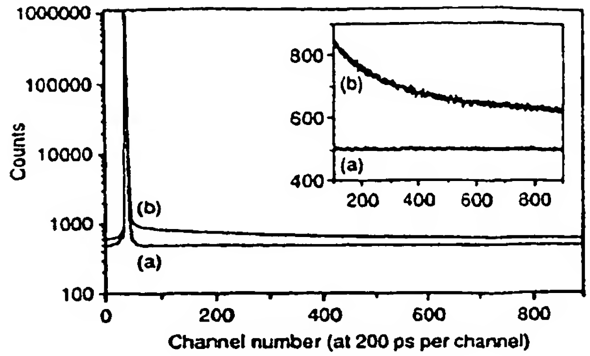

Figure 4 Characteristic lifetime probability density determined using CONTIN for the porous silicon sample taken at 200 ps per channel. (a) Solution 1: zero-time approximately 400 ps beyond the instrumental zero-time channel. (b) Solution 2: zero-time approximately 800 ps beyond the instrumental zero-time channel.

800 ps beyond the instrumental zero-time channel, respectively. Inspection of solution 1 indicates five distinct components. Component 1 is centred at approximately 200 ps and can be attributed to the positrons annihilating either within the silicon substrate or in the remaining silicon in the porous material. Component 2 is centred at approximately 300 ps and has also been encountered by both Itoh *et al.* and Dannefaer *et al.* Their measured lifetimes for component 2, however, ranged between 400 and 600 ps. CONTIN analyses of simulated spectra obeying Poisson statistics indicate that this discrepancy (and the reduced bulk lifetime) may be due to the 200 ps per channel resolution and the neglect of the instrument resolution function. Components 3, 4 and 5, occurring respectively at approximately 2, 10 and 50 ns, are the long lifetime components due to ortho-postronium. In solution 2, the sub-nanosecond components are reduced in intensity, and crystalline silicon and defect components (at 300 ps) are no longer separately resolvable, merging into a single broad peak centred at approximately 250 ps. The long time components now become broader and of a reduced height. This indicates that the widths we have observed are not intrinsic to the material but rather an artefact of the fitting process and the signal to noise ratio. Marshall [14] has concluded that to determine accurately the intrinsic widths of peaks, this ratio must be at least 400. Inspection of Fig. 4 indicates a signal to noise ratio of less than 40 for the positronium decay modes.

The present method of analysis is unsuitable to obtain accurate absolute intensity information since the zero-time channel cannot be estimated beyond the 200 ps per channel limit. Furthermore, modifications to CONTIN suggested by Gregory [12, 15–17] that take into account the finite resolution (and therefore the zero-time channel), by obtaining the probability density profile with respect to a reference spectrum (in our case, bulk silicon), have proved unsuccessful. This is primarily due to the poor definition of the bulk silicon reference spectrum at 200 ps per channel.

Using the PALS data collected from sample A, we have confirmed and extended the findings of both Itoh *et al.* and Dannefaer *et al.* In particular, we resolved three rather than two ortho-positronium components, suggesting that there may be an additional intermediatory scale of porosity in which ortho-postronium annihilates. This has a lifetime indicative of hydrogenated amorphous silicon [18], suggesting ortho-positronium annihilation again within the amorphous layer. The integrated areas (corrected for zero-time shift) of the positronium peaks in solutions 1 and 2 show that components 3 and 5 occur in approximately the same proportion; Dannefaer *et al.*, on the other hand, found that the ~2.5 ns component occurred an order of magnitude less than the longest time ortho-positronium component. The present analysis also establishes the existence of a very weak ortho-positronium component in the pre-anodized wafers at a time scale approximately equal to the longest time ortho-positronium component seen in porous silicon, using theory [19] that has traditionally been employed in the calculation of free volumes in polymer materials. In porous silicon Itoh *et al.* associated a void length scale of approximately 1 nm to this ortho-positronium component, suggesting that irregularities of this magnitude exist on the pre-anodized wafer and that these may, in part, be the catalyst for the initial pore formation process.

The results presented here further demonstrate the rich variety of disorder inherent in porous silicon and indicate the potential of a continuous lifetime analysis of PALS spectra to provide a high resolution probe into such structures. If another order of magnitude increase in signal to noise ratio can be achieved then there exists the possibility of resolving intrinsic peak widths for porous silicon samples, thereby extending the PALS method to resolving pore size distributions using the ortho-positronium components, and conceivably giving insight into the electronic structure of the confined electrons within the remaining silicon crystallites of the porous layer.

Acknowledgements

This work is supported by an Australian Research Council (Large Grant), no. AB9332681 (1994/95). We thank Roman Liebach for the production of the porous silicon sample used in this work.

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Received 1 December 1995
and accepted 5 August 1996

ELSEVIER

Nuclear Instruments and Methods in Physics Research A 384 (1997) 506–515

NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH Section A

Study of the Van Cittert and Gold iterative methods of deconvolution and their application in the deconvolution of experimental spectra of positron annihilation

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Received 15 March 1996; revised form received 11 June 1996

Abstract

The study of deconvolution by Van Cittert and Gold iterative algorithms and their use in the processing of experimental spectra of Doppler broadening of the annihilation line in positron annihilation measurement is described. By comparing results from both algorithms it was observed that the Gold algorithm was able to eliminate linear instability of the measuring equipment if one uses the 1274 keV ^{22}Na peak, that was measured simultaneously with the annihilation peak, for deconvolution of annihilation peak 511 keV. This permitted the measurement of small changes of the annihilation peak (e.g. *S*-parameter) with high confidence. The dependence of γ-ray-like peak parameters on the number of iterations and the ability of these algorithms to distinguish a γ-ray doublet with different intensities and positions were also studied.

1. Introduction

Positron annihilation (PA) as one of the non-destructive nuclear methods is used for the study of structure of different materials and it is especially efficient in determining free volumes or defects in bulk material. The main characteristics, that are determined by PA, are lifetimes of positrons in matter, Doppler broadening of annihilation line (DBAL), and angular correlation of annihilation γ-rays. The last two characteristics give us information about the momentum distribution of electrons in matter. The more common angular correlation method is approximately one order more accurate, but it is more time consuming and requires a more intensive positron source. On the other hand DBAL is simple and not time consuming. It is mainly used for determining the relative changes in the annihilation peak (e.g., *S*-parameter, defined as the ratio between area of central part of the peak to the full area of the peak) depending on temperature, pressure etc. After deconvolution of the annihilation peak using a resolution function of measuring system, one can obtain the momentum distribution of electrons in the sample. If we are only interested in relative changes of the *S*-parameter, deconvolution is not necessary. But as we have seen in our work, deconvolution can partly eliminate the spurious effects due to instability of the measuring system. Another possibility to eliminate an instability of the system is the use of an expensive spectrum stabilizer unit.

Generally, deconvolution algorithms have recently found many applications in various domains of experimental science. They have been applied to such different problems as improving resolution in spectroscopy and measuring the thickness of multilayer structures. There is also the long-standing problem of determination of position and intensities in γ-ray multiplets [1].

2. Theory

The relationship between a measured value $x(t)$ and the raw result of measurement $y(t)$ can be described by a convolution-type integral equation

PII S0168-9002(96)00874-1

$$y(t) = \int_{-\infty}^{\infty} x(\tau)h(t-\tau)\,\mathrm{d}\tau, \tag{1}$$

where $h(t)$ is an impulse response. Knowledge of the instrumental function $h(t)$ is usually required. For a discrete system, Eq. (1) can be written as

$$y(i) = \sum_{k=0}^{N-1} h(i-k)x(k) \qquad i = 0, 1, \ldots, 2N-2, \tag{2}$$

where N is the number of samples of vectors $\boldsymbol{h}$, $\boldsymbol{x}$.

The impulse response has a finite length. Therefore we will assume that $h(i) = 0$ for $i < 0$ and $i \geqslant N$. Then Eq. (2) can be written in a matrix form:

$$\begin{bmatrix} y(0) \\ y(1) \\ y(2) \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ y(2N-2) \end{bmatrix} = \begin{bmatrix} h(0) & 0 & 0 & \cdots \\ h(1) & h(0) & 0 & \cdots \\ h(2) & h(1) & h(0) & \cdots \\ \vdots & \vdots & \vdots & \ddots \\ h(N-1) & h(N-2) & h(N-3) & \cdots \\ 0 & h(N-1) & h(N-2) & \cdots \\ 0 & 0 & h(N-1) & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix} \begin{bmatrix} x(0) \\ x(1) \\ x(2) \\ \vdots \\ x(N-1) \end{bmatrix}, \tag{3}$$

or

$$\boldsymbol{y} = \mathbf{H}\boldsymbol{x}. \tag{4}$$

It means that the columns of $\mathbf{H}$ are represented by vectors $\boldsymbol{h}$ mutually shifted by one position. Multiplying both sides of Eq. (4) by $\mathbf{H}^{\mathrm{T}}$ gives

$$\mathbf{H}^{\mathrm{T}}\boldsymbol{y} = \mathbf{H}^{\mathrm{T}}\mathbf{H}\boldsymbol{x}, \tag{5}$$

or

$$\boldsymbol{y}_1 = \mathbf{H}_1\boldsymbol{x}, \tag{6}$$

where $\mathbf{H}_1$ is Toeplitz matrix [2,3].

Solution of the linear equation system (6) (vector $\boldsymbol{x}$), under the condition that the output vector $\boldsymbol{y}$ and the matrix of the impulse response $\mathbf{H}$ is known, is a problem of deconvolution. The output vector of system $\boldsymbol{y}$ is affected by noise that accompanies each measurement. The existence of this noise strongly affects the process of deconvolution, and can lead to difficulties in solving the linear equation system (6).

The above-formulated problem of input reconstruction is as a rule ill-conditioned, i.e. the estimates $\hat{x}(t)$ of $x(t)$ satisfying Eq. (1) are extremely sensitive to errors in the measured data $y(t)$. It is expressed by the fact, that the matrix $\mathbf{H}_1$ is almost singular. The direct inversion of $\mathbf{H}_1$ for solving $\boldsymbol{x}$ cannot lead to a stable solution. Therefore, in order to solve this problem, the method of regularization must be included. This means that original problem is replaced by an approximate one which solutions are significantly less sensitive to errors in the data $y(t)$.

The Van Cittert iterative method of deconvolution is widely applied in different areas, for example in spectroscopy or in image processing [2,4]. The Van Cittert algorithm of deconvolution is described in detail in Ref. [4], so we will describe it only very briefly.

Its basic form for a general linear discrete system is

$$\boldsymbol{x}^{k+1} = \boldsymbol{x}^{k} + \mu(\boldsymbol{y} - \mathbf{A}\boldsymbol{x}^{k}), \tag{7}$$

where A is system matrix, k represents the number of iterations and μ is the relaxation factor. The convergence condition of Eq. (7) is that the diagonal elements of the matrix A satisfy

$$A_{ii} > \sum_{j=0, j\neq i}^{N-1} A_{ij}, \qquad i = 0, 1, \ldots, N-1. \tag{8}$$

It is obvious that such a diagonal element dominance is rare in physical problems. However, the deconvolution algorithm in Eq. (7) can be modified in a such way that it will satisfy the conditions of convergence. Hence, Eq. (7) becomes

$$x^{k+1} = \mu y + (\mathbf{E} - \mu \mathbf{A}) x^k = \mu y + \mathbf{D} x^k, \tag{9}$$

where E is a unit matrix and

$$\mathbf{D} = \mathbf{E} - \mu \mathbf{A}. \tag{10}$$

Under the condition that $x^0 = \mu$, the successive substitutions give

$$x^k = \mu y + \mu \mathbf{D} y + \ldots + \mu \mathbf{D}^{k-1} y + \mu \mathbf{D}^k y = \mu(\mathbf{E} + \mathbf{D} + \ldots + \mathbf{D}^k) y. \tag{11}$$

Assuming that $\lambda_0, \lambda_1, \ldots, \lambda_{N-1}$ are eigenvalues of A, then $(1-\mu\lambda_0), (1-\mu\lambda_1), \ldots, (1-\mu\lambda_{N-1})$ are eigenvalues of D. If

$$\lim_{k\to\infty} (1-\mu\lambda_i)^k = 0, \qquad i = 0, 1, \ldots, N-1, \tag{12}$$

then

$$\lim_{k\to\infty} \mathbf{D}^k = [0],$$

and

$$\lim_{k\to\infty} x^k = \mathbf{A}^{-1} y = x. \tag{13}$$

From equation (12) this implies that the necessary and sufficient conditions of convergence are

$$|1 - \mu\lambda_i| < 1, \qquad i = 0, 1, \ldots, N-1. \tag{14}$$

If we define λ_i and its conjugate λ_i^* as

$$\lambda_i = a_i + \mathrm{j} b_i, \qquad \lambda_i^* = a_i - \mathrm{j} b_i,$$

then the convergence condition (14) becomes

$$\mu[\mu(a_i^2 + b_i^2) - 2a_i] < 0, \qquad i = 0, 1, \ldots, N-1. \tag{15}$$

Inequality (15) gives two bounds for μ

$$\mu = 0, \qquad \mu = 2\frac{a_i}{a_i^2 + b_i^2}, \qquad i = 0, 1, \ldots, N-1. \tag{16}$$

N conditions determine the bounds of the μ coefficient. Unfortunately these conditions are not fulfilled for all cases. However, if the system matrix A is positive definite the convergent solution always exists. So we settle the algorithm in a such way that the eigenvalues λ_i will be positive, real numbers.

Let us return to Eq. (5). Matrix $\mathbf{H}^T\mathbf{H}$ is symmetric, so its eigenvalues are real. The eigenvalues of matrix $(\mathbf{H}^T\mathbf{H})(\mathbf{H}^T\mathbf{H})$ are squares of eigenvalues of matrix $\mathbf{H}^T\mathbf{H}$ and therefore must be positive. Eq. (5) becomes

$$(\mathbf{H}^T\mathbf{H}\mathbf{H}^T) y = (\mathbf{H}^T\mathbf{H}\mathbf{H}^T\mathbf{H}) x, \tag{17}$$

and the iterative algorithm of deconvolution becomes

$$x^{k+1} = x^k + \mu[(\mathbf{H}^T\mathbf{H}\mathbf{H}^T)y - (\mathbf{H}^T\mathbf{H}\mathbf{H}^T\mathbf{H})x^k], \tag{18}$$

or

$$x^{k+1} = x^k + \mu[y' - \mathbf{H}'x^k]. \tag{19}$$

By this we ensure the existence of a common interval of solution for inequality (14) and convergence of the deconvolution algorithm. Eigenvalues λ_i are real, positive numbers, so from Eq. (16) for μ we can write

$$0 < \mu < \frac{2}{\lambda_{max}}, \tag{20}$$

where λ_{max} is the greatest eigenvalue of $\mathbf{H}'$

$$\lambda_{max} = \max(\lambda_0, \lambda_1, \ldots, \lambda_{N-1}). \tag{21}$$

Now we determine the maximum eigenvalue λ_{max}. For eigenvalues of system (17) we can write

$$\mathbf{H}'x = \lambda_i x, \qquad i = 0, 1, \ldots, N-1. \tag{22}$$

If x_j is the biggest absolute element in x, then from Eq. (22) we get

$$\sum_{m=0}^{N-1} \mathbf{H}'_{jm} x_m = \lambda_i x_j \tag{23}$$

or

$$\lambda_i = \frac{\sum_{m=0}^{N-1} \mathbf{H}'_{jm} x_m}{x_j}. \tag{24}$$

Then

$$\lambda_i \leqslant \sum_{m=0}^{N-1} |\mathbf{H}'_{jm}|, \qquad i = 0, 1, \ldots, N-1. \tag{25}$$

In practical cases we do not know the biggest element in x. We determine the value of λ_{max} as the maximum value from λ_i, determined by Eq. (25) e.g., from the sum of absolute values of rows in matrix $\mathbf{H}'$.

This is the base of the Van Cittert algorithm of deconvolution. Now we introduce, in analogy with Eq. (24), a local variable relaxation factor

$$\mu_i = \frac{x_i^k}{\sum_{m=0}^{N-1} \mathbf{H}'_{im} x_m^k}, \tag{26}$$

and we use it in Eq. (19). For the ith element of vector x^{k+1} we get

$$x_i^{k+1} = x_i^k + \frac{x_i^k}{\sum_{m=0}^{N-1} \mathbf{H}'_{im} x_m^k}\left[y_i - \sum_{m=0}^{N-1} \mathbf{H}'_{im} x_m^k\right]. \tag{27}$$

or

$$x_i^{k+1} = \frac{y_i}{\sum_{m=0}^{N-1} \mathrm{H}'_{im} x_m^k} x_i^k . \tag{28}$$

Eq. (28) is the Gold algorithm of deconvolution [5]. It is an extension of Van Cittert's iterative method. The advantage of Gold's method is that the solution x is positive.

3. Theoretical simulation

To test an applicability of Van Cittert's and Gold's methods of deconvolution for γ-rays spectra we performed a theoretical simulation. We convoluted the experimental resolution function (RF) obtained from a positron annihilation experiments with different kinds of Gaussians describing γ-ray peaks. The simulated spectra were used as an input to both Gold's and Van Cittert's iterative deconvolution procedures. Simulated spectra included a noise component due to an experimental resolution function.

3.1. The dependence of output peak parameters from the deconvolution on the number of iterations

Because the deconvolutions are using the iterative method, it was interesting to study the dependence of the output from the deconvolution on the number of iterations (N). N was varied in the range 200–50000. 2000 iteration steps lasted 40 min on a PC486, 33 MHz for 200 channels of the spectrum (a version with elimination of the multiplication of zero matrix terms took approx. 15 min).

We analyzed the peak which was a convolution of a Gaussian with FWHM = 13 channels and a resolution function with a FWHM = 10.4. The resulting peak had a FWHM = 16.7, which was a value in the range of our experimental values for the FWHM of annihilation peaks measured in DBAL. The deconvoluted peak was fitted and the result should be one Gaussian with a FWHM = 13.

Fig. 1 shows the dependences of the χ^2 value and FWHM on the number of iterations for the algorithm of Van Cittert and Gold. As we can see from this figure, the resulting deconvolution fit for the Van Cittert algorithm was much better for two Gaussians than for one until 14000 iterations, then the χ^2 became practically the same.

For the Gold algorithm the χ^2 of the deconvolution fit was very good for one Gaussian and reached a minimum value for 2000 iterations. The increase of χ^2 with the number of iterations (for both Van Cittert and Gold methods) is a consequence of the round-off errors which arise during the computations with real numbers represented in standard single precision (REAL in Fortran or FLOAT in C) and a large number of these

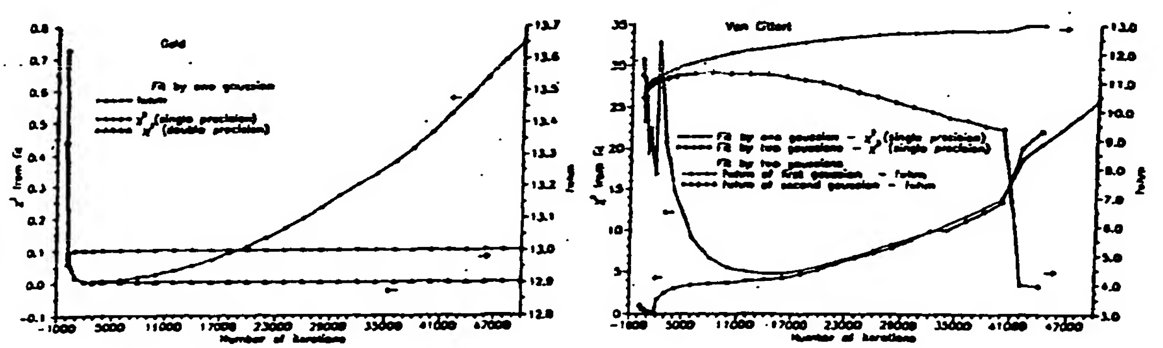

Fig. 1. Dependence of χ^2 and FWHM from fit of deconvoluted peak on number of iteration steps.

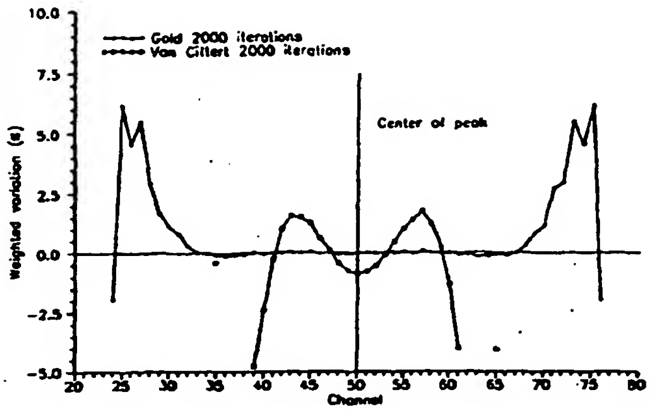

Fig. 2. Weighted variations of deconvoluted peak and original Gaussian.

operations. It was verified by a calculation (for the Gold method) using the double precision floating-point representation of real numbers. The results of the double-precision calculation are shown in Fig 1. The fast convergence and the stability of the solution can be observed. It clearly shows the possible errors arising from using a finite computer word length of and a large number of iteration steps.

For the Van Cittert algorithm, it can be seen that by increasing the number of iterations the first Gaussian became more and more dominant and approached the input Gaussian in convolution. The same dependence can be observed in the intensity of Gaussians.

For the Gold algorithm, the results were much better. From Fig. 1, it is clear that the FWHM from the fit of the deconvoluted peak reached the correct value of 13 for the number of iterations larger than 1000. The variance of the FWHM from this fit was $< 0.03\%$ and of the amplitude $< 0.005\%$ for $N \geqslant 1000$.

For the Van Cittert algorithm and $N \geqslant 2000$, the variance of the FWHM from the fit was $< 0.3\%$ and of the amplitude $< 0.05\%$.

In Fig. 2 the weighted differences of the original input Gaussian and fitted results of the deconvoluted peak after $N = 2000$ iteration steps are shown. The difference is evident. For the Gold deconvolution the variance was still less than 7.5% even for the ±25 displaced channels from the center of the peak. For the large number of iterations ($N > 30\,000$) there was already deformation in deconvoluted peak, which could be seen as sharp peaks in the dependence of weighted differences. This deformation is a consequence of round-off errors in the computer.

Fig. 3 shows typical results of the deconvolution procedures. The peak, deconvoluted by the Gold's algorithm, is almost identical with the original Gaussian after carrying out 2000 iterations. Van Cittert's procedure showed negative values and there were oscillations on both wings of the peak on the level of 2% of amplitude of peak. Because Fig. 3 is in a logarithm scale the negative values are not displayed. Gold's deconvolution did not produce negative values and oscillations were very small ($< 0.01\%$).

3.2. *The deconvolution of Gaussians with different FWHM*

To determine the influence of the FWHM of the convoluted Gaussian on the result of deconvolution, we also made a convolution of the Gaussian with FWHM = 20 with RF. Then the difference in parameters of the resulting deconvoluted peak after 2000 iterations was compared with the difference for FWHM = 13.

The Van Cittert's deconvolution of convolution of the original Gaussian with a FWHM = 20 was in very good agreement with the original Gaussian, χ^2 from the fit was 0.04 and the FWHM was exactly the same.

The weighted difference of the fit of deconvoluted and original Gaussian was $\leqslant 10\%$ for counts $> 0.1\%$ of amplitude. The situation was worse for the convolution of the Gaussian with FWHM = 13. The FWHM of the deconvoluted peak was larger than about 1.8%. But the worst fact was that the χ^2 from the fit was

very large (Fig. 1) and the deconvolution was better described by two Gaussians ($\chi^2 = 1.8$). That means that the deconvolution changed the shape of the peak in such a way that the deconvoluted peak could be better described by two Gaussians though there should be only one. The weighted difference of the deconvolution fit and the original Gaussian was $\leqslant 10\%$ for counts $> 3\%$ of the amplitude. The parameters from the fit of deconvoluted peak were in excellent agreement with the original Gaussian. Problem was that for a Gaussian with FWHM = 13 there was a better χ^2 for two Gaussians as for one.

For the Gold deconvolution agreement with the original Gaussian was very good also for Gaussian with FWHM = 13 as we can see from Fig. 2. What was important was that there are no deformations in deconvoluted peak because the χ^2 for one Gaussian was very small (Fig. 2).

3.3. The deconvolution of the sum of two Gaussians with different intensity and position

To verify the possibility of distinguishing components of a doublet (sum of two peaks) by deconvolution, we made convolutions of the sum of two Gaussians with intensity ratios 1:1, 1:0.8, 1:0.5, 1:0.2 and mutual displacements of 1, 5, 10, 15, 20 channels. Both input Gaussians had FWHM = 13, the number of iteration steps N was 2000 and the deconvoluted peaks were fitted. We computed the weighted difference of these fitted parameters with the parameters of the original input Gaussians.

For the Van Cittert's deconvolution we got the following results:

If the peak displacement was 15 and 20 channels there was no problem to fit the deconvolution results. The variation from the parameters of the input Gaussians was small, $\leqslant 2\%$. For a displacement of about 10 channels, the fitting procedure for the ratio of intensities 1:0.2 failed. The variance was $\leqslant 5\%$ for ratios 1:1, 1:0.8 and $< 19\%$ for 1:0.5. For a displacement of about 5 channels we were not able to get a fit for 1:0.2 and 1:0.5 ratios. The variances were $< 42\%$ (the largest for the amplitude, for the remaining parameters $< 10\%$). So for peak displacements larger than the FWHM of the peaks, the resolution was good also for the ratio of intensity of 20%. For a displacement smaller as the FWHM of the peak, the resolution was possible only for intensities close to each other. For a small displacement ($< 10\%$), the fit was impossible.

For the Gold deconvolution we also got a fit for a displacement of 10 channels and ratio 1:0.2 and a displacement of 5 channels and ratios 1:0.5, 1:0.2 with variances $< 27\%$. For a displacement of 1 channel the fitting procedure failed. So we can say that Gold's algorithm is much more able to distinguish a doublet and give us more precise results than the Van Cittert's algorithm.

In Fig. 4 convolutions of Gaussians and the results of the deconvolution procedure described above can be seen.

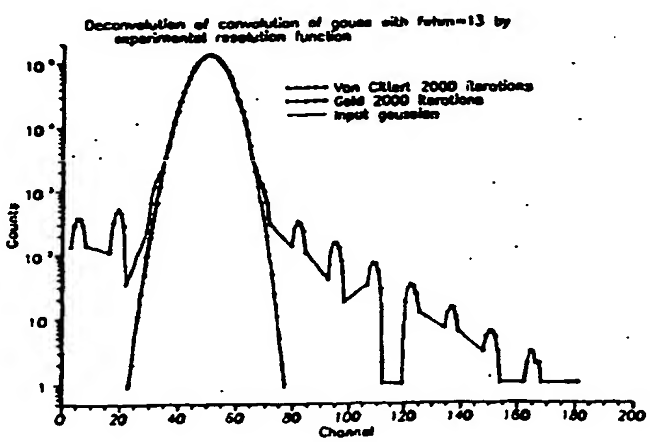

Fig. 3. Comparison of peak deconvoluted by Van Cittert and Gold method.

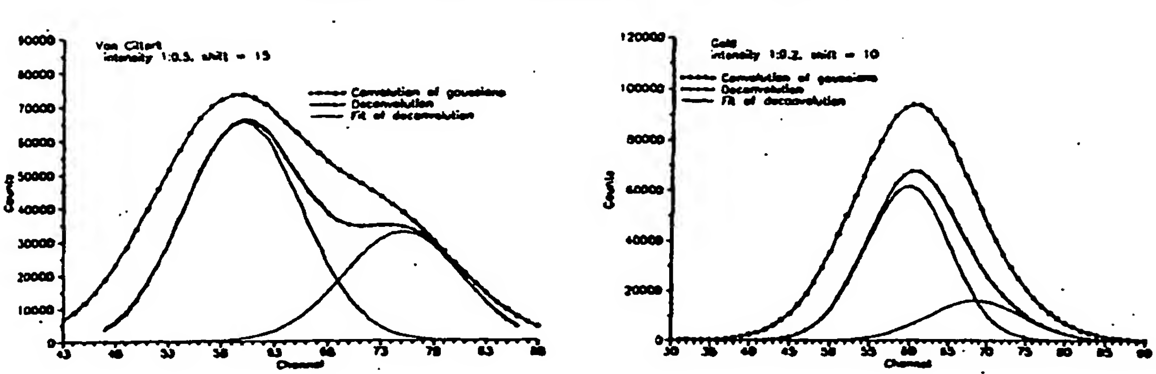

Fig. 4. Convolution and deconvolution of Gaussians.

4. Experimental spectra

All these studies of the convolution of Gaussians and following deconvolution were aimed at finding out the possibility and limitations of the deconvolution methods and their possible use in the deconvolution of experimental γ-ray spectra. Because the methods are quite reliable (especially Gold's method) we have used Gold's deconvolution method for our experimental spectra.

The effect of DBAL is quite smallscale and one needs a very stable measuring system for its measurement. We can get information about its stability from the 1274 keV peak, which is measured simultaneously with the 511 keV annihilation peak if we use ^{22}Na as a radioactive source.

In our experiment we used an HPGe detector with a resolution of 1.56 keV at 570 keV with a ^{207}Bi source. The energy calibration of the system was 163 eV/channel. The number of counts at the annihilation peak was ≈630 000 and the number of counts at the 1274 keV peak was ≈180 000. In Fig. 5 we can see the *S*-parameter with physical information about the momentum distribution of the electrons and the *S*-parameter of the 1274 keV peak, which carries information about the stability of the measuring system. If there was no instability during the measurement, it should be a constant. As we can see, the *S*-parameter of the 1274 keV peak was not constant, so the measuring system was not stable. So we do not know if the structure in the *S*-parameter of 511 keV peak was really a consequence of this instability or if it had a real physical meaning. Of course, there is a possibility to try to use the *S*-parameter of the 1274 keV peak as a correction on the instability, e.g. by calculating the ratio $R = S(511\ \text{keV})/S(1274\ \text{keV})$. The result of such procedure is shown in Fig. 5. As we can see, this simple procedure does not suppress the effect of instability. Because we are

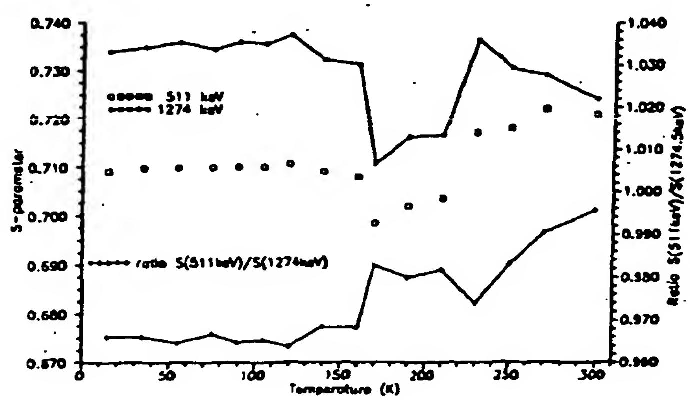

Fig. 5. *S*-parameters without the deconvolution procedure and the ratio *R* of the *S*-parameter at 511 keV to the *S*-parameter at 1274 keV.

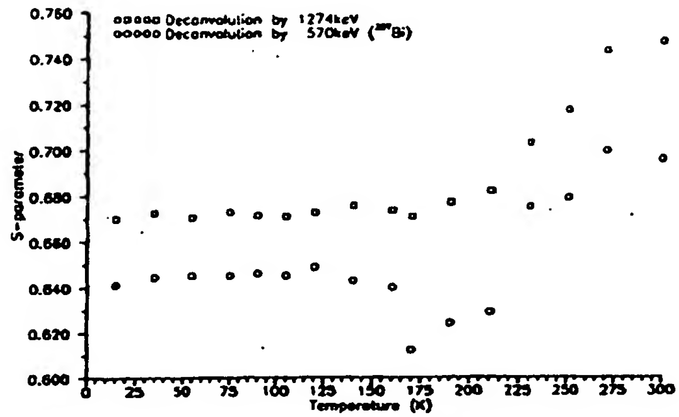

Fig. 6. S-parameters after deconvolution.

interested only in the relative changes of the S-parameter on temperature, we can make a deconvolution of the 511 keV peak with the 1274 keV peak and try to suppress the effect of instability.

Fig. 6 shows the result of these deconvolutions (the S-parameter after deconvolution) along with the S-parameter from deconvolutions of the 511 keV peak with the 570 keV peak (^{207}Bi), which was measured at the beginning of our experiment. So we can see that the structure at the temperature of 175 K was only a consequence of instability of the measuring system, because it disappeared after the deconvolution of the 511 keV peaks with the 1274 keV peaks. We can obtain physical information from the dependence of the S-parameter on the temperature by using a deconvolution procedure.

This procedure can also be used for a reliable estimate of the electron momentum distribution. In such case we need a better resolution function (e.g. 514 keV from the decay of ^{85}Sr) measured simultaneously with the annihilation line.

5. Conclusion

It turned out that the described deconvolution methods are in principle convenient for processing experimental spectra from DBAL measurements. They help to sup press influence of instability of the measuring system. Particularly the Gold deconvolution method works very well and it does not deform the deconvolution result. The reproducibility of the deconvolution results tested on simulated convolutions of Gaussians is very good. Van Cittert's algorithm gives the results with oscillations from positive to negative values on the wings of the deconvoluted peaks. Gold's deconvolution gives only small non-negative oscillations. Unambiguously we can say that Gold's algorithm is more reliable with regard to the precision of the deconvolution. The time needed for the deconvolution is practically the same for both algorithms.

So, the use of Gold deconvolution is a cheap and simple way to eliminate the electronic instabilities which blur physical effects.

Acknowledgements

This work was supported by the Grant Agency of Slovak Republic in part under contract No. 2/2035/95. The authors would like to thank the referee for his helpful comments on this problem.

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